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LASER EYE PROTECTION GROUPWARE APPLICATION INFORMATION SYSTEM

by
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PREFACE

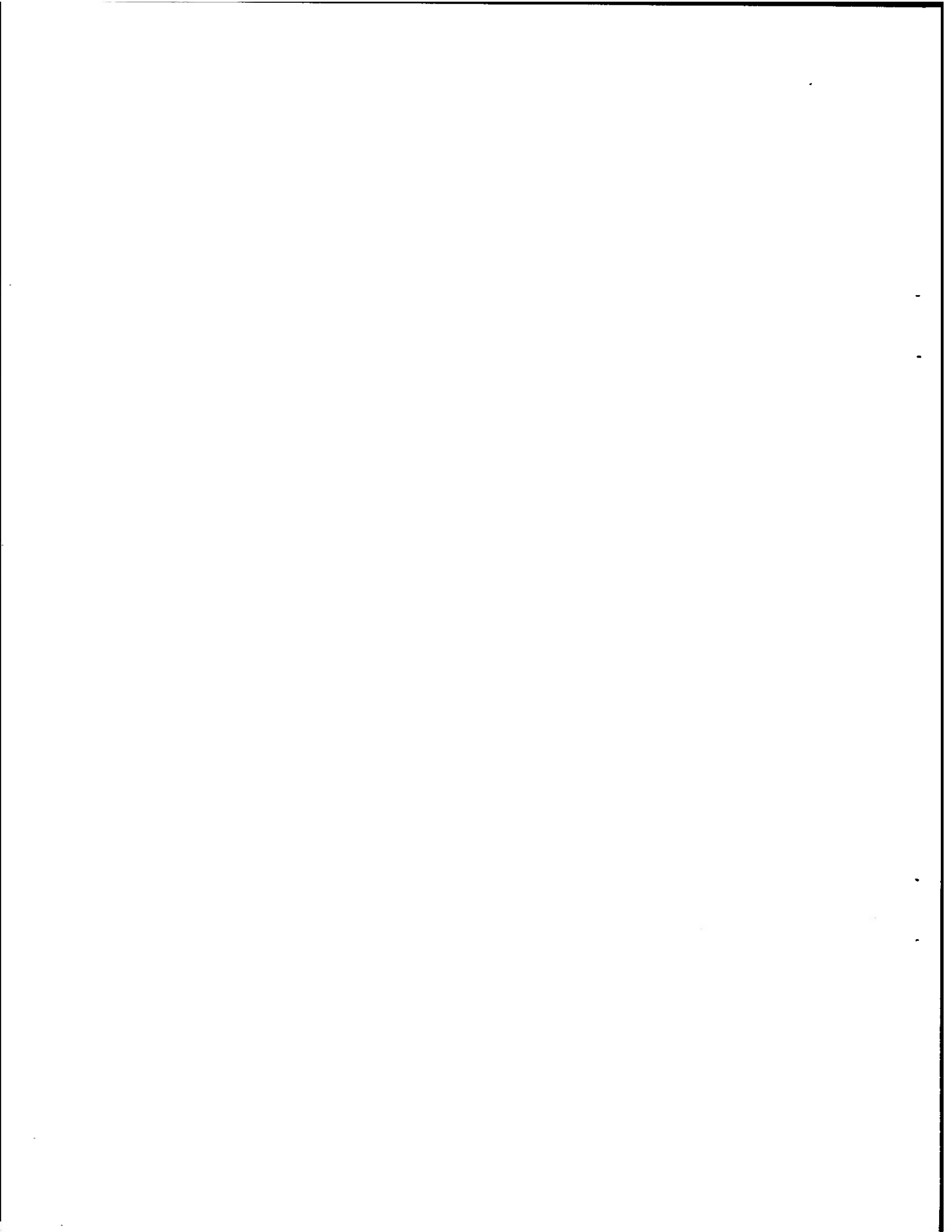
The authors appreciate the advice of Mr. Jeffery Redding, Lotus Notes Administrator at Natick, MA, Soldier Systems Center of US Army Soldier and Biological Chemical Command, who provided technical expertise in designing the database.

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LASER EYE PROTECTION GROUPWARE APPLICATION INFORMATION SYSTEM

I. INTRODUCTION

An effective information system is becoming increasingly more important for a research effort, such as laser eye protection, to be competitive, timely, and complete as the quantity and availability of scientific data proliferates. An IS can be a crucial component of success to assess how our research correlates with the LEP research field as a whole. In a February 1997 review of Natick Research, Development, and Engineering Center's (NRDEC's) LEP by the organization's Senior Technical Advisory Council (STAC), the STAC recommended an enhanced accessibility of our in-house data. This recommendation provided the motivation to establish the information system.

In order to establish an IS, it was necessary to identify an appropriate software platform. Requirements were that the software be easy to use, provide flexibility so that it could easily be adapted to LEP information, and that our entire team be able to access and edit information.

Lotus Notes belongs to an application category of database software called groupware. The purpose of this type of software is to organize information and make it easily available to individuals working together who may need the information for different purposes. For LEP research, a requirement might be to identify compounds with the largest $\chi^{(3)}$ values. On the other hand, the requirement might be to identify for each compound the wavelength of the maximum absorption peak, λ_{\max} . Another requirement could be to identify all publications in the database that include Professor D. V. G. L. N. Rao as an author. Lotus Notes provides a mechanism to easily access and compare a variety of types of information with numerical and text fields such as these.

Our team's initial considerations included selecting specific types of information to access in the database. Previous research efforts of our team had encompassed the entire directed energy area (including LEP) and also the thermal area. We decided to focus on the topic of our current in-house research in laser eye protection. Our external collaborations for the laser eye work are also included. For this information resource to be complete, in-house reference materials for the areas of microwave protection and thermal protection are also included so that all of our information resources are documented in one place and can be computer searched together. However, the only actual numerical data that are organized and sorted by the database are related to LEP. Consequently, the database is named the Laser Eye Protection Database.

Another relevant issue was the lack of previous experience using Lotus Notes for most team members. Therefore, it was essential to learn how to use this software. Up-to-date resource materials were acquired (1 - 8) and used for reference.

Another step in establishing the IS was to contact the Natick Notes Administrator, Mr. Jeffery Redding, for assistance. Mr. Redding's help was required as a Lotus Notes technical expert and database designer.

The architecture of the IS is shown in Figure 1. The LEP Lotus Notes database resides on a Natick server. All LEP team members can create new files and edit information. All Natick LAN users can read the information in the database. A general description of the database is provided on the server for new users. This documentation is Appendix A.

This report describes some features which have been incorporated into this IS and demonstrates the capabilities of this system to facilitate a research effort such as LEP.

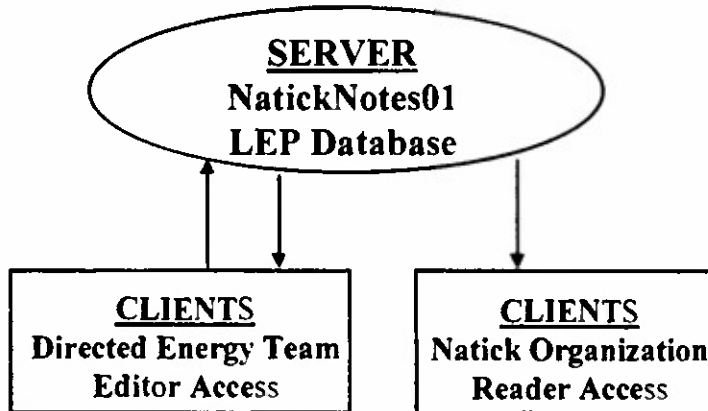


Figure 1. Architecture of LEP Client/Server Information System

II. BASIC STRUCTURE OF LASER EYE PROTECTION DATABASE

A. Forms and Fields

Information in the database is organized by using forms. Each different form in the database is designed to optimize the organization of a specific type of data. This Lotus Notes database has two types of forms. The most prevalent form is the "Chemical Report". The other type of form is "Program and Data Files". This is a blank form that is included as a repository for attachments with experimental data provided to plot linear absorption spectra.

Information is entered into this Lotus Notes database by filling in the blanks of the "Chemical Report" forms just as information is entered on a hard copy form. After information has been added to a form and saved, the form is then referred to as a document. Therefore a document is defined as a completed form.

The "Chemical Report" form is shown in Figure 2. The name of a nonlinear optical material was designated as the most important piece of information and so the title of each document is the name of a chemical compound. User input fields are the blanks to which data are added and are indicated by upper left and lower right hand brackets. There are twenty-two user input fields in this form.

In addition to fields into which information can be added, there are also fields where information cannot be inputted by users because they were designed into the form. These "static" fields are in the areas outside the two sets of brackets. Some examples of static fields for the "Chemical Report" form are the headings "Concentration" and "Solvent" and are shown in Figure 2 below.

Chemical Report		Chemical Compound:
05/11/98		Entered By: Linda Holtz
Concentration:	g/ml	Solvent:
Comments:		
Extinction Coefficient:		Chl-3:
Comments:		Comments:
Second Hyperpolarizability:	esu	Ground State Cross-Section:
Comments:		cm2
Excited State Cross-Section:	cm2	Absorption Peak:
Comments:		esu
References Title:		
Source:		
Date:		
Author:		
Structure:		
Additional Information:		
**** Include data path, nlsnotes, c:\msdos\win31		

Figure 2. "Chemical Report" Form and Associated User Input and Static Fields

B. Documents

The fundamental element of a Lotus Notes database is the document. The documents of the "Chemical Report" format are described below.

Since each document is constructed of distinct fields, an important initial step in designing the database was to identify appropriate fields for the "Chemical Report" form. The goal was to answer the question: *What specific information is required to characterize each individual nonlinear optical material?* Each user input field contains a designated type of information (e.g., text, numeric). In the LEP Database, there are 15 primary user input fields and they are: Chemical Compound, Concentration, Solvent, Extinction Coefficient (ϵ), Third Order Macroscopic Susceptibility ($\chi^{(3)}$), Second Hyperpolarizability (γ), Ground State Cross-Section (σ_0 or σ_{gr}), Excited State Cross-Section (σ_{ex}), Absorption Peak (λ_{max}), Reference Title, Source, Date, Author, Structure, and Additional Information (see Figure 2).

Some of these primary user input fields have an additional associated Comment field for inclusion of information which is supplementary. For example, the Concentration field has a Comment field associated with it. There are 7 secondary Comment fields and these are also shown in Figure 2. These Comment fields provide additional pertinent information. For example, if there is more than one absorption peak, the wavelength of the strongest peak, λ_{max} , can be included in the "Absorption Peak" field and the additional information specifying the wavelength(s) of any weaker absorption peak(s) can be included in the associated "Absorption Peak - Comments" field. The 15 primary input fields plus the 7 secondary Comments fields comprise the 22 user input fields shown in Figure 2. A document for zinc meso-tetra-(p-dimethylaminophenyl)-tetrabenzporphyrin is shown in Figure 3 as an example.

There is not a separate primary user input field for the nonresonant (single photon) two photon absorption coefficient, β . Values for β are included in the secondary comments field for the ground state cross section.

The magnitude of $\chi^{(3)}$ is contained in the primary "Chi-3" field. If the real and imaginary parts of $\chi^{(3)}$ are known, this additional information is provided in the secondary "Chi-3 Comments" field.

The information in document fields facilitates quick visual comparisons of data pertaining to one specific nonlinear optical material under a specified set of experimental conditions. For example, the magnitudes of the excited state cross-section and the ground state cross section can be compared by examination of a document. Since the excited state absorption mechanism correlates with $\sigma_{ex} > \sigma_0$, this is a useful comparison. Also, comparisons can be made between the magnitudes

of the real and imaginary parts of $\chi^{(3)}$. For optical limiting and laser eye protection the magnitude of the imaginary part of $\chi^{(3)}$ predominates over the magnitude of the real part and this information is contained in the document.

Each of the documents of the "Chemical Report" type is associated with a molecular structure of interest evaluated under one specific set of conditions in laser eye protection research. For example, there is a document for the chemical compound zinc meso-tetra-(p-dimethylaminophenyl)-tetrabenzporphyrin.

If one particular molecular compound was evaluated under different experimental conditions, then there would be more than one document for this molecular structure; there would be one document for each set of experimental conditions.

A couple of the primary user input fields are rich text fields. This means that essentially any type of data format may be used, including pictures or attachments. For example, in the "Structure" field some chemical compound structures are included as Windows metafile (.wmf) icon attachments. When the attachment is viewed, the chemical structure is displayed. The other rich text field is the "Additional Information" field. Any type of supplemental information may be included in this field. Hot links have been included in some of the "Additional Information" fields to facilitate quick access to another document that contains relevant information. Also, if the document contains data from a technical report or journal article, an abstract may be provided in this field. Abstracts can provide useful information in a document to facilitate searches of the database.

Chemical Report
04/16/97

Chemical Compound: ZN MESO-TETRA-(P-DIMETHYLAMINOPHENYL) TBP
Inputted By: Linda Hoke

Concentration:	g/mL	Solvent:	THF
Comments:	range of concentrations evaluated between E-05 g/mL and E-04 g/mL.		
Extinction Coefficient:		Chi-3:	2.80E-08 esu
Comments:		Comments:	
Second Hyperpolarizability:	1.00E-29 esu	Ground State Cross- Section:	cm ²
Comments:		Comments:	
Excited State Cross- Section:	cm ²	Absorption Peak:	4.50E+02 nm
Comments:		Comments:	450 nm (strong) 640 nm (weak)
Reference Title:	Third-order, nonlinear optical interactions of some benzporphyrins		
Source:	Applied Physics Letters		
Date:	03/91		
Author:	Rao, D.V.G.L.N.; Aranda, Francisco J.; Roach, Joseph F.; and Remy, David E.		

Structure: Zinc meso-tetra-(p-dimethylaminophenyl)tetrabenzporphyrin:

Chemical structure diagram: Laser Eye Protection Database (Natick Labs Hardcopy)

Additional Information: (could include data plots, pictures, comments, etc.)

- method: DFWM (532 nm)
- solution transparent in green region
- 17 ps pulse width
- 25 mJ average pulse energy
- nonlinearly predominately electronic in origin (versus nuclear orientation in origin)

ABSTRACT

We measured third-order, nonlinear optical susceptibility χ^3 for a series of tetrabenzporphyrins in solution in tetrahydrofuran at 532 nm using degenerate four-wave mixing with picosecond pulses and obtained values of molecular second hyperpolarizability, γ . The corresponding macroscopic χ^3 values calculated for nine compounds with different substituent groups are four to five orders larger than χ^2 . For five of the compounds the χ^3 values are in the range $1.2 - 2.8 \times 10^{-8}$ esu. Our experiments indicate that the nonlinearity is predominately electronic in origin with a response time faster than the 15 ps resolution of our system.

Figure 3. Document for Zinc Meso-Tetra-(p-Dimethylaminophenyl) Tetra-benzporphyrin

C. Views

A view provides a mechanism to organize and sort information. The design of the views in this database is crucial to the utility of the database. A question to be answered when designing views is: *What comparisons are important among different nonlinear optical materials in the database?* Identifying the view categories was a crucial step in planning the database. This database has twelve views: Absorption, Author, Chemical Compound, Chi-3, Concentration, Data & Program Files, Excited State Cross-Section, Extinction Coefficient, Ground State Cross-Section, Reference, Reference Date, and Second Hyperpolarizability. The menu of these views is shown in Figure 4 as it appears on the computer screen in Lotus Notes. The views are listed in ascending order alphabetically.

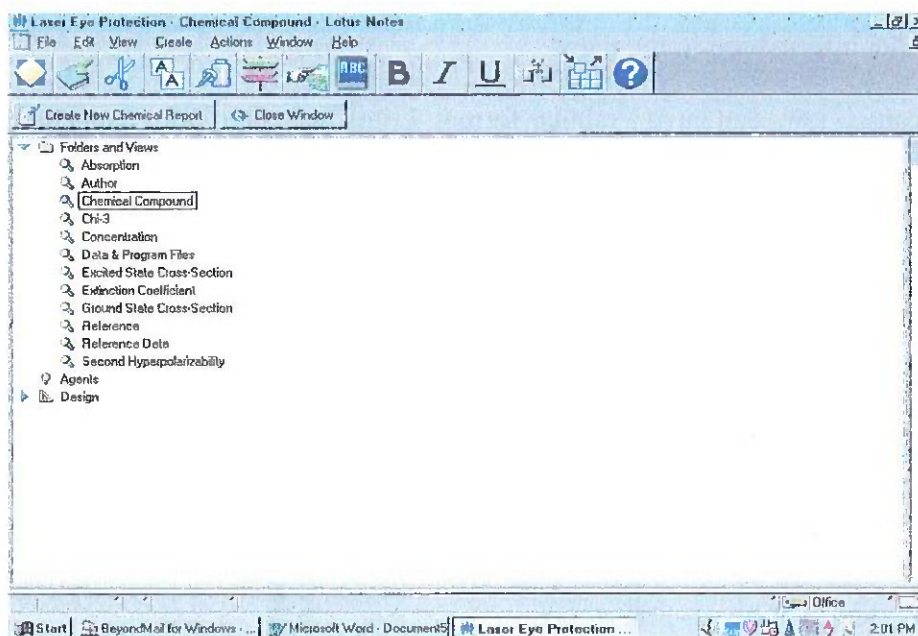


Figure 4. Menu of Laser Eye Protection Database Views

Among the types of questions which can be easily and quickly answered by using views are: "Which materials have the largest $\chi^{(3)}$ values?"

When searches are conducted, it is the separate views that are searched. Not all documents appear in every view. This is an important consideration when performing searches for information contained in the database. The view which contains all the

documents in the database is "Chemical Compound" (shown selected in Figure 4). Therefore, this view provides access to all documents in the database when conducting searches.

Information in a view is presented in tabular form and can be sorted and/or categorized by various criteria. Multiple levels of categorization can be displayed in each view. The views in this database have up to four levels of categorization. The first categorized column in a view sorts the data by values within that column and displays the results in hierarchical format. This creates different levels of information with the first column being the highest level. Subsequent categorized columns are displayed at lower levels. The complete document is always located at the lowest level. This structure allows the user the luxury of seeing data pertinent to his or her search without having to open each full document.

When starting at the highest (or first) level and sequentially accessing additional columns of the view table from left to right, users can obtain additional details which help clarify the information in the view.

Because views can have a tabular format, Lotus Notes provides a mechanism to create spreadsheets from views. Not all information in a view will necessarily be incorporated into a spreadsheet. The user can select the desired information. This utility can be helpful for preparing reports and presentations. In addition, spreadsheet contents can easily be displayed graphically.

The levels structure is illustrated in Figure 5. The levels structure and corresponding tabular format for each individual view will be explained in the following sections.

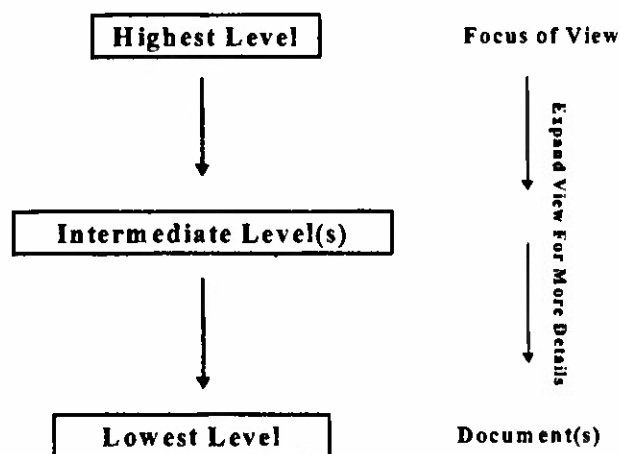


Figure 5. Levels Structure of Database Views

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1. Absorption View

In the absorption view the primary criterion is the wavelength of the absorption maximum, λ_{\max} . This view has two levels. The first level is shown as the first column and lists the magnitudes of λ_{\max} values. This column has the heading "nm". The second level of this view consists of two columns with headings "Chemical Compound" and "Comments". The "Comments" column has additional information about the linear absorption of the nonlinear optical material. This view is shown schematically in Figure 6A. and as it actually appears in Lotus Notes in Figure 6B.

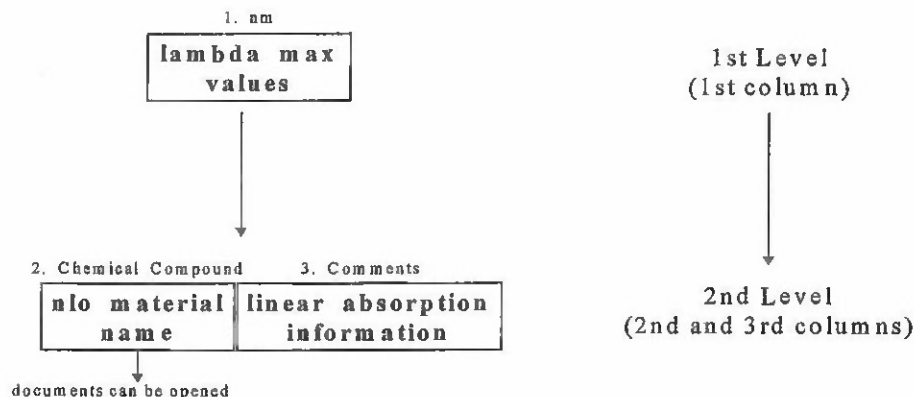


Figure 6A. Absorption View Schematic

nm	Chemical Compound	Comments
	Bipolaronic 7-BTP	Bipolaronic n-BTPs (n = 6 to n=9, where n = number of conjugated double bonds) have an absorption peak between 610 nm and 870 nm (specific data for Bipolaronic 7-BTP not provided)
	Bipolaronic 8-BTP	Bipolaronic n-BTPs (n = 6 to n=9, where n = number of conjugated double bonds) have an absorption peak between 610 nm and 870 nm (see Fig. 3 of Reference for absorption spectrum of Bipolaronic 8-BTP)
	Bipolaronic 9-BTP	Bipolaronic n-BTPs (n = 6 to n=9, where n = number of conjugated double bonds) have an absorption peak between 610 nm and 870 nm (specific data for Bipolaronic 9-BTP not provided)
▼ 450	Mg octamethyl-TBP	450 nm (strong) 640 nm (weak)
	TBP	450 nm (strong) 640 nm (weak)
	Zn hexadecafluoro-TBP	450 nm (strong) 640 nm (weak)
	Zn meso-tetra-(p-fluorophenyl)-TBP	450 nm (strong) 640 nm (weak)
	Zn meso-tetra-(p-dimethylaminophenyl)-TBP	450 nm (strong) 640 nm (weak)
	Zn meso-tetra-(p-methoxyphenyl)-TBP	450 nm (strong) 640 nm (weak)
	Zn meso-tetra-methyl-TBP	450 nm (strong) 640 nm (weak)
	Zn meso-tetraphenyl-TBP	450 nm (strong) 640 nm (weak)
▼ 390	PPQ	second peak 280 nm with shoulder at 300 nm; concentration for absorption measurement: 1.0E-05g/mL

Figure 6B. Absorption View Computer Screen

2. Author View

The primary category for this view is the name of the first author of a technical report or journal article. This view has three levels. The first level consists of one column and lists the name(s) of the author(s) sorted by last name of first author. The second level consists of the second column and lists two pieces of information. The first is the publication date (mm/dd/yy) and the second is the title of the article. The third level consists of the third column which lists the names of the nonlinear optical materials. This view is shown schematically in Figure 7A. The three levels as they actually appear in Lotus Notes are shown in Figures 7B, 7C, and 7D.

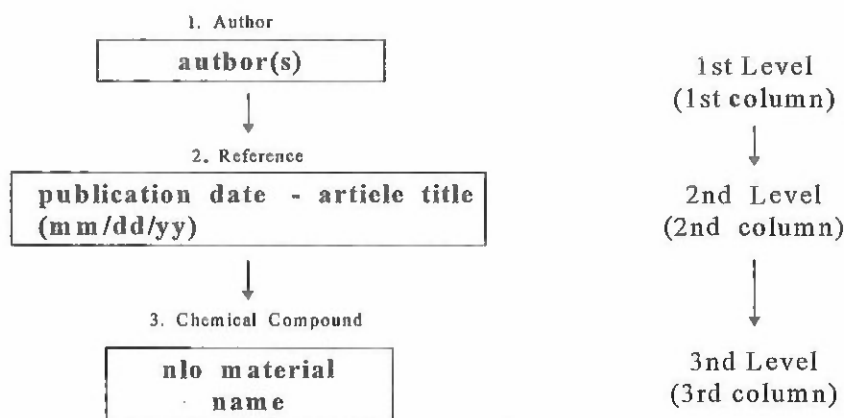


Figure 7A. Author View Schematic

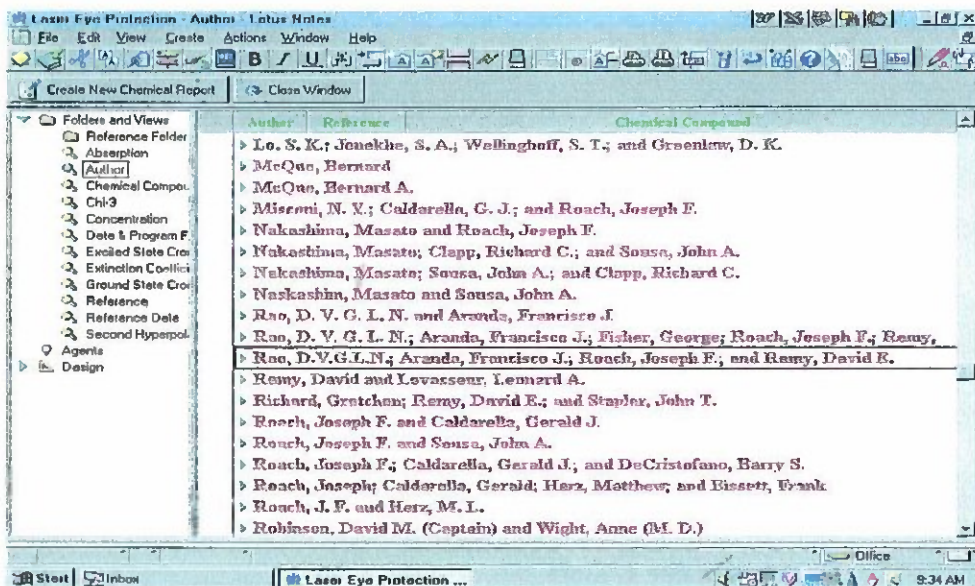


Figure 7B. First (Highest) Level of Author View Sorted in Ascending Alphabetical Order by Last Name of First Author

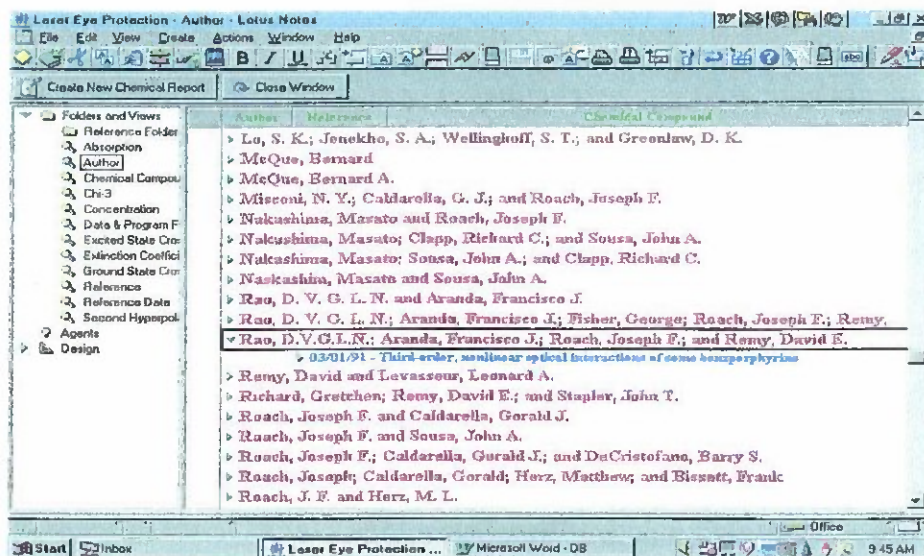


Figure 7C. Second Level of Author View Providing Publication Date and Article Title

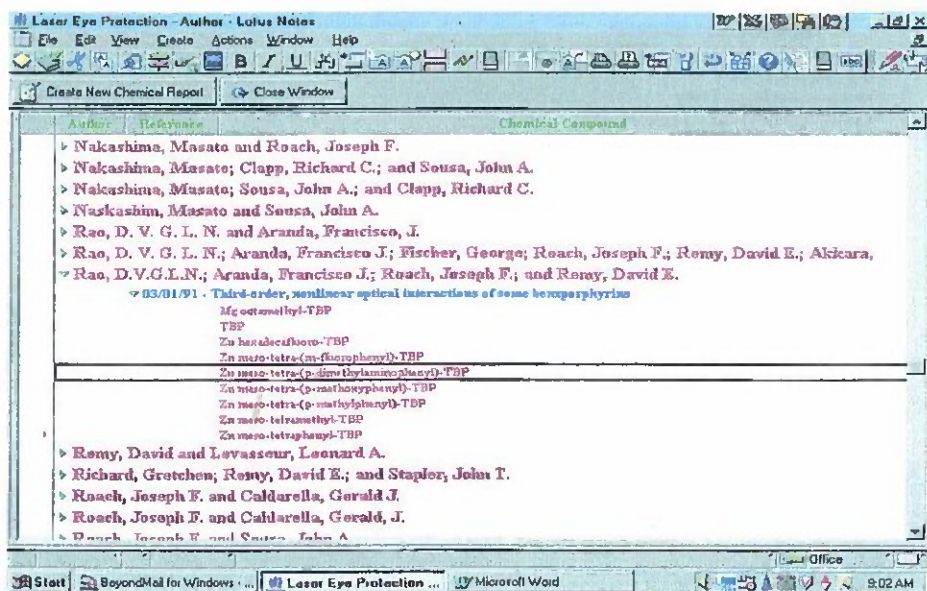


Figure 7D. Third Level of Author View Showing Document Titles as Chemical Compound Names in Ascending Order. Opening Selected Document Produces Figure 3.

3. Chemical Compound View

This view lists and sorts all the names of all the nonlinear optical materials in the LEP database. Some materials appear more than once because these materials have been evaluated using different experimental conditions and there is a document for each set of conditions. This view has one level. This is the most fundamental view in the database because it contains all the documents. Therefore, this may be an optimum view to use when conducting searches of the database. This view is shown schematically in Figure 8A and as it actually appears in Lotus Notes in Figure 8B. If there are document attachments, a paperclip icon appears in the first column. There is one level with one column.

1. Chemical Compound

nlo material name

Figure 8A. Chemical Compound View Schematic

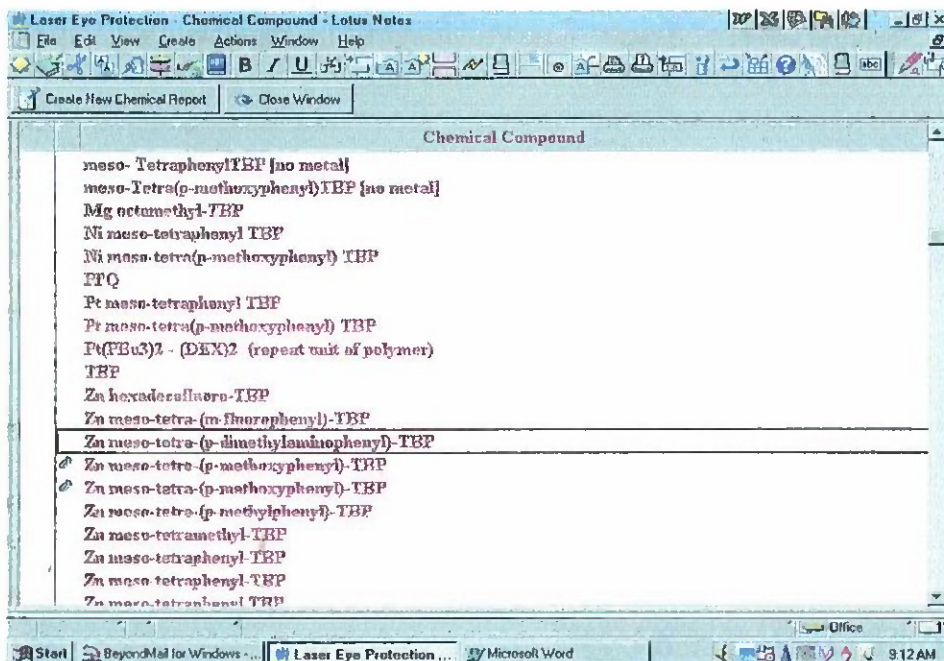


Figure 8B. Chemical Compound View Computer Screen. If the Selected Document is Opened, Figure 3 is Obtained.

4. Chi-3 View

The primary sorting category for this view is the value of the macroscopic third order susceptibility, $\chi^{(3)}$, of nonlinear optical materials in units of esu. This view has two levels. The second level consists of two columns. One of the columns lists the names of the nonlinear optical materials. The second column provides comments with supplementary information about the $\chi^{(3)}$ of a material, including the real and imaginary parts, if known. This view is shown schematically in Figure 9A and as it actually appears in Lotus Notes in Figure 9B.

To determine the nonlinear optical material that has the largest $\chi^{(3)}$ value, first access the Chi-3 view. The values of $\chi^{(3)}$ are sorted in descending order, so that by inspection, the largest value is 2.8×10^{-8} esu for Zn meso-tetra-(p-dimethylaminophenyl) TBP.

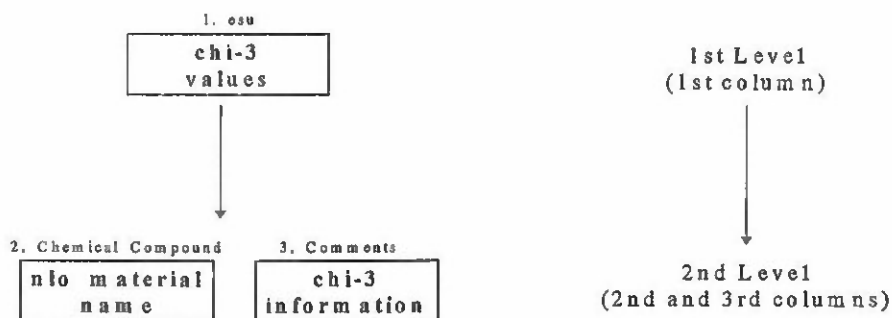


Figure 9A. Chi-3 View Schematic

esu	Chemical Compound	Comments
(Not Categorized)	PPQ	real part: 8.1E-10esu imaginary part:1.6E-09 esu
	Pi(PBu3)2 - (DEX)2 (repeat unit of polymer)	real part: 26 (+/- 3) E-14 esu imaginary part: 13 (+/- 1.2) E-13 esu
	Zn meso-tetra-(p-methoxyphenyl)-TBP	real part: 7.8 (+/- 3.5) E-14 esu imaginary part: 9 (+/- 1) E-13 esu
	Zn meso-tetraphenyl-TBP	real part: 9.1 (+/- 4.5) E-14 esu imaginary part: less than or equal to 1.8E-13 esu
2.80E-08	Zn meso-tetra-(p-dimethylaminophenyl) TBP	
1.50E-08	Zn meso-tetramethyl-TBP	
1.40E-08	Zn meso-tetra-(p-methoxyphenyl)-TBP	
1.30E-08	Zn meso-tetra-(m-fluorophenyl)-TBP	
1.20E-08	Zn meso-tetra-(p-methylphenyl)-TBP	
8.00E-09	Mg octamethyl-TBP	
3.00E-09	TBP	
2.00E-09	Zn meso-tetraphenyl-TBP	
1.00E-09		

Figure 9B. Chi-3 View Computer Screen. If the Selected Document is Opened, Figure 3 is Obtained.

5. Concentration View

This view provides the numerical value of the concentration in g/mL for a nonlinear optical material in solution. There are two levels and three columns. The second level lists the name of the nonlinear optical material and the solvent. This view is shown schematically in Figure 10A and as it appears in Lotus Notes in Figure 10B.

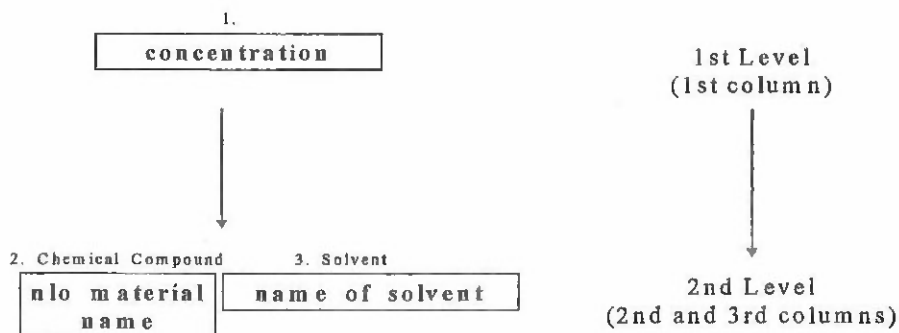


Figure 10A. Concentration View Schematic

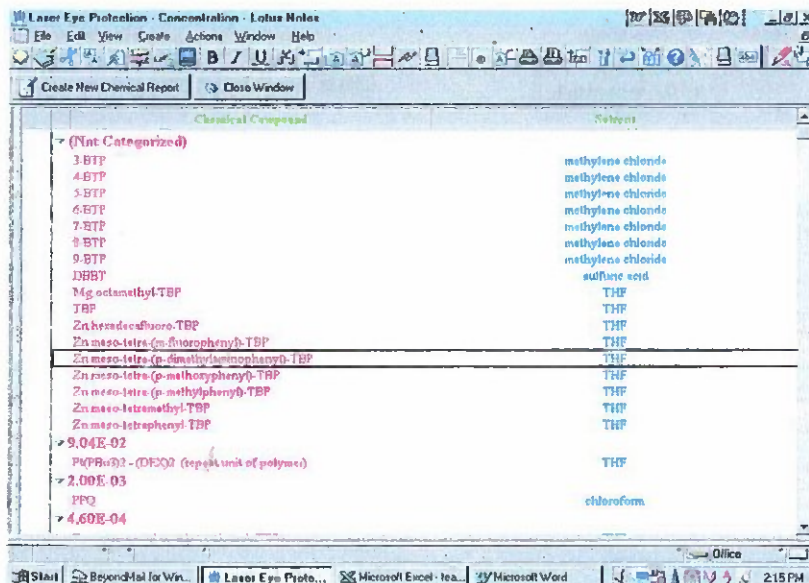


Figure 10B. Concentration View Computer Screen. If Selected Document is Opened, Figure 3 is Obtained

6. Data & Program Files View

This view does not have a levels structure but is an unformatted view, which is a repository for data files for linear absorption spectra.

7. Excited State Cross-Section View

The main category of this view is the excited state cross section in units of cm^2 . This view has two levels. The second level has two columns, which are the nonlinear optical materials' names and supplementary information pertaining to the excited state cross section. This view is shown schematically in Figure 11A and as it appears in Lotus Notes in Figure 11B.

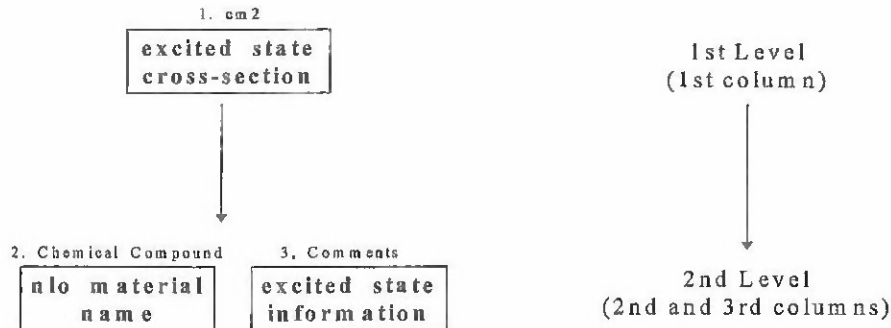


Figure 11A. Excited State Cross-Section View Schematic

Compound Name	Excited State Cross-Section (cm^2)
DBBT	1.03E-17 cm^2 (see comments)
Zn meso-tetraphenyl TBP	7.2000000000E-17
Cu meso-tetra(p-methoxypheno) TBP	4.3000000000E-17
Pt meso-tetraphenyl TBP	3.4000000000E-17
Zn meso-tetra(p-methoxypheno) TBP	3.0000000000E-17
Zn meso-tetraphenyl TBP	+/- 0.25E-17 cm^2
Ni meso-tetra(p-methoxypheno) TBP	+/- 0.25 E-17 cm^2
Pt meso-tetra(p-methoxypheno) TBP	2.3000000000E-17
Ni meso-tetra(p-methoxypheno) TBP	2.1000000000E-17
Ni meso-tetraphenyl TBP	1.6000000000E-17
Pt(PBu3)2-(DEX)2 (repeat unit of polymer)	1.0000000000E-17
	+/- 0.25-17 cm^2

Figure 11B. Excited State Cross-Section View Computer Screen

8. Extinction Coefficient View

This view has two levels. The highest level is for the value of the extinction coefficient. There is no title heading for this level. The second level has two columns with headings "Chemical Compound" and "Comments". Information under these headings would be the name of the chemical compound and comments pertaining to the extinction coefficient.

9. Ground State Cross-Section View

This view has the same structure as the excited state cross section view and is shown in Figures 12A and 12B. Notice in Figure 12B that the nonresonant two photon absorption coefficient β appears in the Comments field.

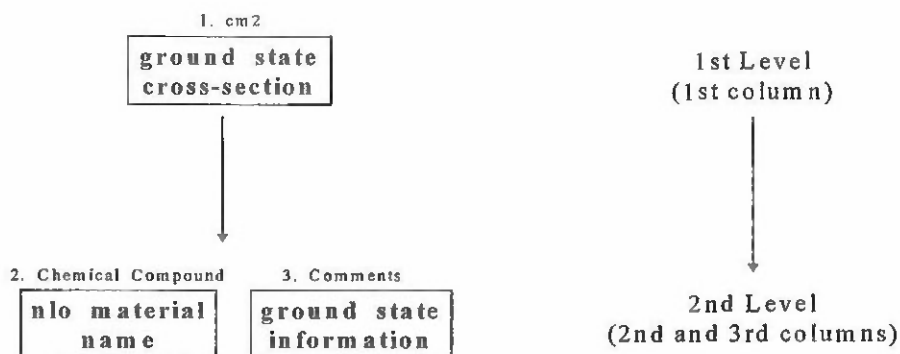


Figure 12A. Ground State Cross-Section View Schematic

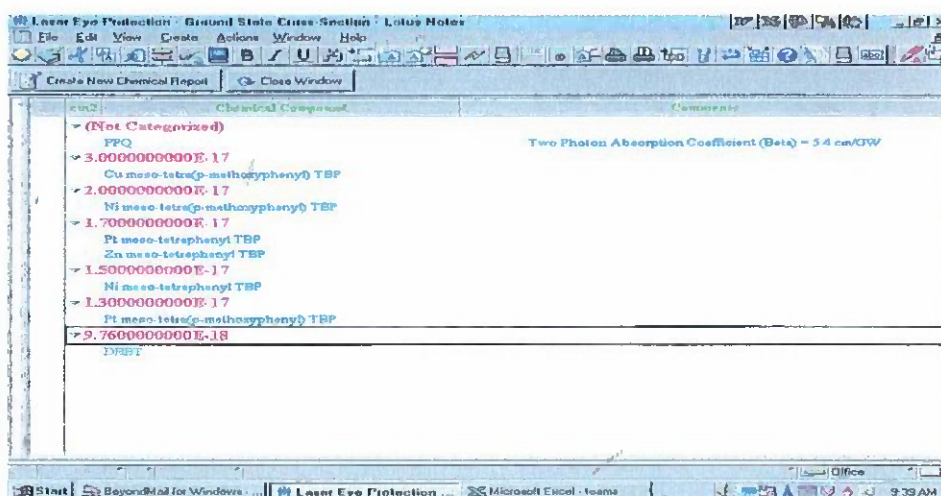


Figure 12B. Ground State Cross-Section View Computer Screen

10. Reference View

The main information in this view is the title of a technical report or journal article. This view has three levels. Figures 13A and 13B illustrate the Reference view.

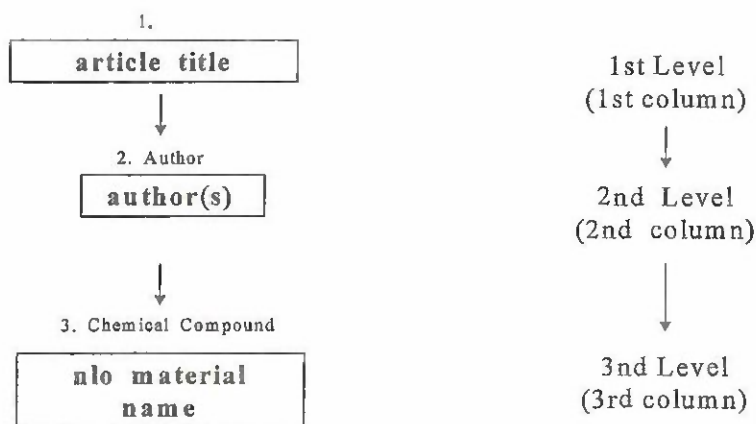


Figure 13A. Reference View Schematic

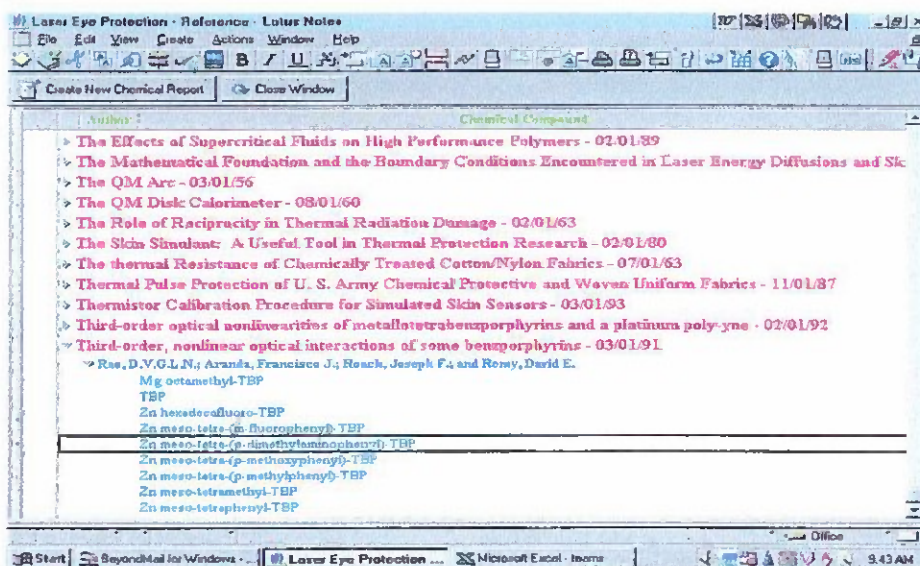


Figure 13B. Reference View Computer Screen. If Selected Document is Opened, Figure 3 is Obtained

11. Reference Date View

The reference date view is illustrated in Figures 14A and 14B.

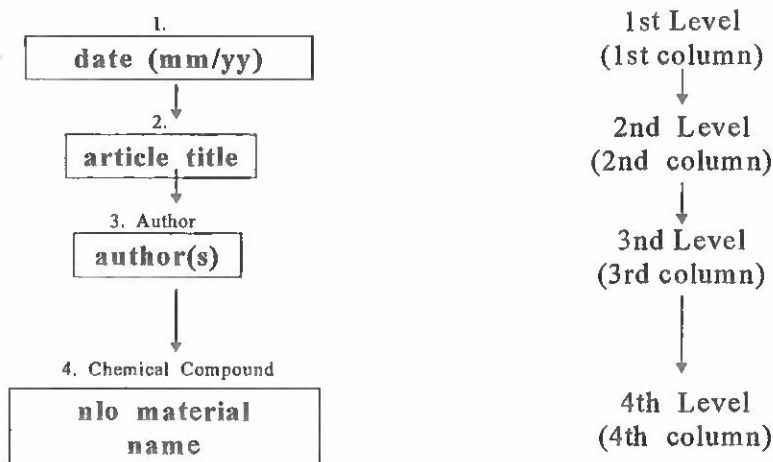


Figure 14A. Reference Date View Schematic

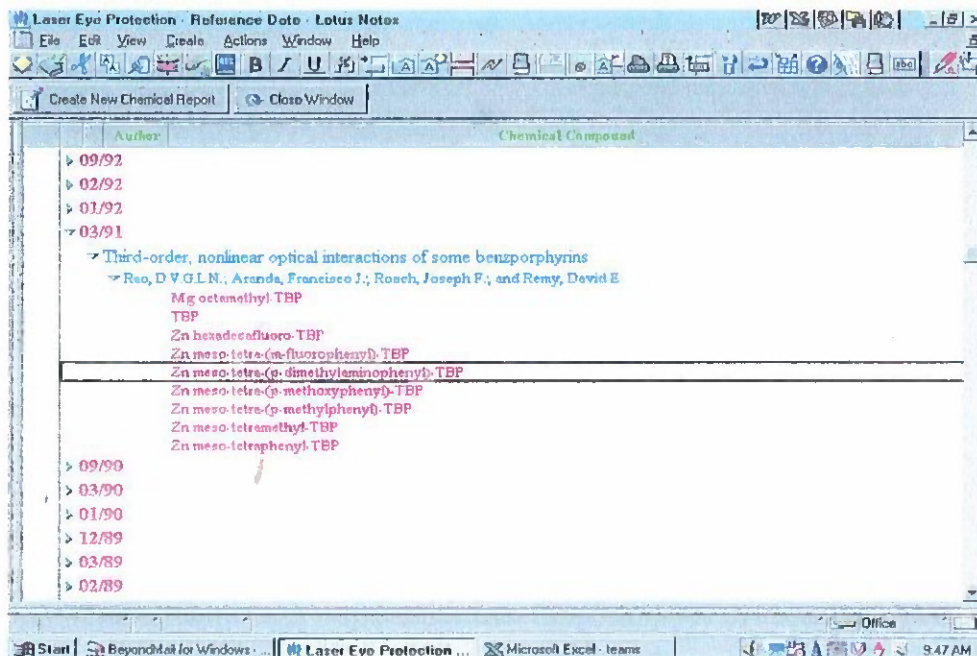


Figure 14B. Reference Date View Computer Screen. If Selected Document is Opened, Figure 3 is Obtained.

12. Second Hyperpolarizability View

The second hyperpolarizability view is illustrated in Figures 15A and 15B.

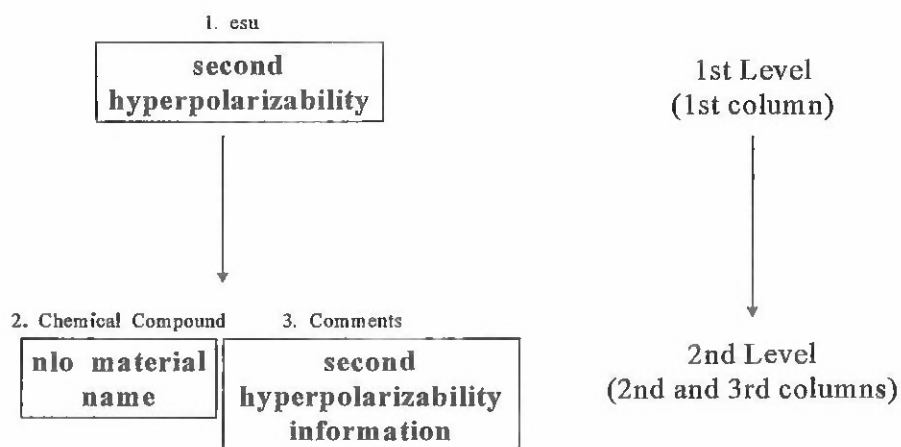


Figure 15A. Second Hyperpolarizability View Schematic

esu	Chemical Compound	Comments
1.14E-28	Bipolaronic 9-BTP	+/- 50%
5.10E-29	9-BTP	+/- 50%
3.19E-29	Bipolaronic 8-BTP	+/- 50%
2.35E-29	9-BTP	+/- 50%
1.50E-29	7-BTP	+/- 50%
1.00E-29	Zn meso-tetra-(p-dimethylaminophenyl)-TBP	
8.70E-30	6-BTP	+/- 50%
4.80E-30	Zn meso-tetra-(p-methoxyphenyl)-TBP	
4.00E-30	Zn meso-tetra-(p-methylphenyl)-TBP	
3.80E-30		
3.30E-30		
2.45E-30		

Figure 15B. Second Hyperpolarizability View Computer Screen. If Selected Document is Opened, Figure 3 is Obtained.

III. FINDING INFORMATION QUICKLY

In addition to providing the mechanism of views to access information, Lotus Notes has sophisticated search features. The most comprehensive search is a full text search using a view that has the most documents in it. That view is the Chemical Compound view. In some cases, selecting a view with fewer documents may help limit and focus a search. To support searches, the LEP database is full-text indexed.

The operators AND, OR, and NOT are available for searching. In addition, exact phrases may be searched by including them in quotes. Furthermore, each of the 22 fields of the "Chemical Report" form can be individually searched (Figure 2). To achieve searches of individual fields, select "Add Condition" (adjacent to the text entry box on the Search Bar) and use the Search Builder dialog box. (Appendix B provides information that can be useful for detailed searches of this database.)

For example, to identify the publications where Professor D. V. G. L. N. Rao was an author, the "Author" input field could be searched. It would not be necessary for Professor Rao to be first author for a publication to be selected. Whenever a search term such as "Rao" is found in a document, it is enclosed in a red box to help the user understand the search results.

Other search utilities in Lotus Notes include determining the relevance of the documents found in the search and ranking the documents with the greatest relevance first. The number of times a search word appears or the proximity of search words in documents may be used as criteria for relevance ranking.

IV. MACRO FOR PLOTTING ABSORPTION SPECTRA

One of us (MN) has written a Microsoft Excel[®] macro to plot linear absorption spectra using data collected for nonlinear optical materials by use of the $\lambda 9$ spectrophotomer. This macro along with instructions for its use and also data files (.dx files included as attachment icons) are included as a part of the database.

The macro or program file is included in the database as an attached EXCEL file (.xls), denoted by an icon in the Program & Data Files document. The user clicks twice on this icon to obtain a properties dialog box. Three options are provided: (a) View Option which lists the instructions required to run the EXCEL macro, (b) Launch Option which opens EXCEL and the macro file if EXCEL is installed on the user's PC, and (c) Detach Option which copies the macro to the user's hard disc drive for future use with the EXCEL software without accessing Lotus Notes software first. An example absorption spectrum plot is shown in Figure 16 below.

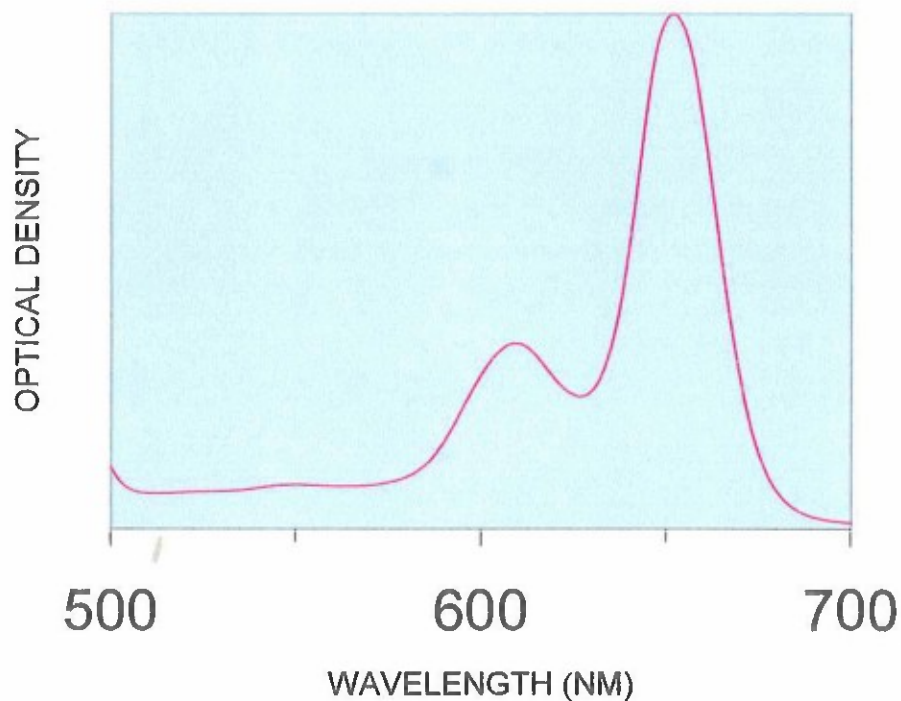


Figure 16. Absorption Spectrum Plot

V. HOT LINK FEATURES

Links are provided in some documents to go quickly to other documents with relevant information. For this database all links are included in the "Chemical Report" form in the Additional Information field. These links all go to the "Data & Program Files" document where appropriate data are provided to plot the linear absorption spectrum of a nonlinear optical material.

VI. POTENTIAL FOR INTERNET CONNECTION

Lotus Notes 4.5 has its own browser or Notes Navigator so that it is possible to access the Internet from Lotus Notes. Therefore it is possible to incorporate a URL as a hotspot link so that a WWW page could be accessed directly while using Lotus Notes. One of the goals in establishing this database was to create an information resource that would serve as a tool to facilitate the planning of our research in LEP. In order to make the most meaningful contributions, it is crucial that we communicate and collaborate with others in this area of research. This database focuses on in-house data and collaborations. However, the potential exists to link directly from Lotus Notes to appropriate WWW pages and access information from other researchers in the LEP field.

VII. CONCLUSION

A Lotus Notes database such as this one on laser eye protection has the potential to greatly facilitate research progress when a team works together to achieve a common goal. The capacity to access, sort, compare, and evaluate quickly and easily appropriate information using a variety of different formats has the potential to provide insights and serve to provide guidance for future research.

Using the link features and navigator could greatly expand the capabilities of this information system. The architecture previously shown in Figure 1 could be modified as shown in Figure 16.

This effort served as an example of how to set up a groupware type of information resource for scientists working in the area of LEP. Using Lotus Notes software as a central component of our information system did achieve our goals of providing a user-friendly information resource, which can provide a resource for preparation of reports and presentations and furthermore facilitate planning and evaluation of research results.

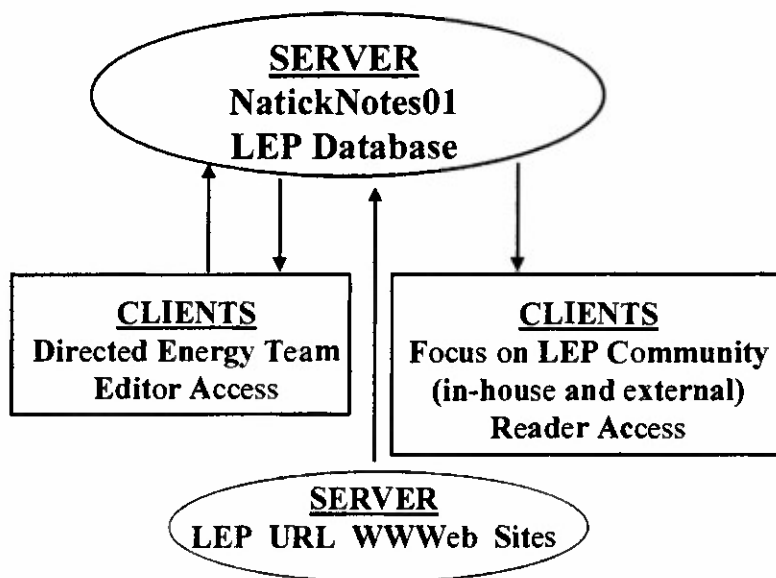


Figure 17. Modified Architecture of LEP Information System

VIII. REFERENCES

1. Cates, Richard, **Using Lotus Notes and Domino 4.5**, QUE Corporation, 1997.
2. Rayl, Eric, **Lotus Notes Developer's Guide**, SAMS Publishing, 1994.
3. Marmel, Elaine, **Easy Lotus Notes 4.5**, QUE Corporation, 1997.
4. Brown, Kenyon; Brown, Kyle; Koutchouk, Francois; and Brown, Kevin, **Mastering Lotus Notes 4.5 and Domino**, Sybex, Inc., 1996.
5. Collin, Simon, **A Complete Guide to Lotus Notes 4.5**, Digital Press, 1997.
6. Plumley, Sue, **10 Minute Guide to Lotus Notes 4**, QUE Corporation, 1996.
7. Kelleher, Rose; Emond, Paul; and Jones, Tom, **Lotus Notes Developer's Guide**, Wordware Publishing, Inc., 1997.
8. Kreisle, Bill, **Lotus Notes 4.5**, MIS:Press, 1997.

APPENDICES

APPENDIX A. USING THE DATABASE DOCUMENT

I. VIEWS

This database consists of 10 views: absorption, author, chemical compound, chi-3, concentration, excited state cross-section, ground state cross-section, reference, reference date, second hyperpolarizability. Each of these views may be selected by clicking once on the appropriate item under the Folders and Views Category.

These views provide different methods to access information pertaining to nonlinear optical materials. The chemical compound view lists all materials contained in the database in alphabetical order. If an item (nonlinear optical material) which is displayed in this view is clicked once, it is selected. If an item is clicked twice, its document is opened.

As an example of how to use a view as a strategy to obtain desired information, consider the chi-3 view, which displays all the chi-3 values of all the materials in the database. This view lists these values in descending order so that the largest chi-3 values are at the beginning of the list. The nonlinear optical material associated with a specific chi-3 value can be identified by clicking on that chi-3 value, which prompts Lotus Notes to display the name of the material.

As another example, the reference date view lists all of the publication dates of the references used for information for the database. These dates are listed in descending order so that the most recent dates appear at the top of the list. If a date is selected, then the reference title is provided. Further clicking on items of interest will result in additional information being provided. In this case, the authors and finally the specific nonlinear optical materials evaluated in this reference can be obtained.

APPENDIX A. USING THE DATABASE DOCUMENT (CONT'D)

II. DOCUMENTS

Each nonlinear optical material has a document in the database. The document contains detailed information pertaining to a specific nonlinear optical material. Some examples of the types of information which documents may contain are: chemical structure diagrams, experimental method used to obtain nonlinear optical data, solvent used, solute concentration, chi-3 value, ground and excited state cross sections, absorption peak(s), plot of the absorption spectrum, source of information (journal article or technical report, author(s), date).

III. ADDITIONAL INFORMATION

The functional POC for the database is Landa Hoke (508) 233-4588.

Other editors of the database are: Barry DeCristofano (508) 233-4255, Masato Nakashima (508) 233-5515, Brian Kimball (508) 233-4375.

The technical POC for this database is Jeff Redding (508) 233-5895.

APPENDIX B. FIELDS FOR USE IN FULL TEXT SEARCHES

AbComments

Contains information about the absorption peaks. For example, peaks other than λ_{\max} might be provided here. [Comments] (under **Absorption Peak**)

Absorption

Provides the wavelength of the main absorption peak, λ_{\max} , in nanometers (nm). [Absorption Peak]

Author

Provides the author(s) of a technical report or journal article. The format is: last name, first name initial(s). [Author]

Chi3

Provides the value of the third-order macroscopic susceptibility, $\chi^{(3)}$, in electrostatic units (esu). [Chi-3]

ChiComments

Contains information pertinent to the third-order macroscopic susceptibility other than the actual value of $\chi^{(3)}$. [Comments] (under **Chi-3**)

Comments

In the "Chemical Report" form, this is the last field in the document. [Additional Information]

Compound

Provides the name of the nonlinear optical material. [Chemical Compound]

DateCreated

Provides the date that a Chemical Report was created (MM/DD/YY).

ECComments

Provides information pertaining to the extinction coefficient, ϵ . [Comments] (under **Extinction Coefficient**)

ESComments

Provides additional information pertaining to the excited state cross-section, σ_{ex} . [Comments] (under **Excited State Cross-Section**)

ESCross

Provides the value of the excited state cross-section, σ_{ex} , in units of cm^2 . [Excited State Cross-Section]

APPENDIX B. FIELDS FOR USE IN FULL TEXT SEARCHES (CONT'D)

Extinction

Provides the value of the extinction coefficient, ϵ . [**Extinction Coefficient**]

Form

There are two types of *forms* or templates for this *database*. For most of the *documents* the *form* name is "Chemical Report". The second type of *form* which is contained in this *database* is named "Program and Data Files". There is only one *document*, which is based on this second template.

GSComments

Provides information about the ground state cross-section, σ_o or σ_{gr} , other than the actual value. [Comments] (under **Ground State Cross-Section**)

GSCross

Contains the value of the ground state cross-section, σ_o or σ_{gr} , in units of cm^2 . [**Ground State Cross-Section**]

Hyper

Contains the value of the second-order microscopic hyperpolarizability, γ , in electrostatic units (esu). [**Second hyperpolarizability**]

InputtedBy

Provides the name of the person who created the *document*.

Reference

Contains the title of a technical report or journal article. [**Reference Title**]

ReferenceDate

Provides the date of publication of the technical report or journal article. The format is MM/YY. [**Date**]

SHComments

Provides uncertainties for the second-order microscopic hyperpolarizabilities, γ_s . [Comments] (under **Second Hyperpolarizability**)

SHDeviation

Same as SHComments

SolComments

Provides information pertaining to the solution of the nonlinear optical material in addition to the value of the concentration and the name of the solvent. [Comments] (under **Concentration**)

APPENDIX B. FIELDS FOR USE IN FULL TEXT SEARCHES (CONT'D)

Solubility

Contains the concentration of the nonlinear optical material in units of g/mL.

[**Concentration**]

Solvent

Contains the name of the solvent used for the nonlinear optical material. [**Solvent**]

Source

Provides the technical report number or the name of the journal. [**Source**]

Structure

Provides the chemical structure of the nonlinear optical material. This is a *rich text field*.

[**Structure**]

Untitled

This is the *rich text field* for the "Program and Data Files" *form*. [**Program and Data Files**]

APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA

```

Attribute VB_Name = "Module1"
Sub Mact()
Attribute Mact.VB_ProcData.VB_Invoke_Func = " \n14"
    macfilent
    Macro1
    Macro6
    Macro7
    Macro8
    Macro9
    Macro10
    Macro11
End Sub
Sub macfilent()
Attribute macfilent.VB_ProcData.VB_Invoke_Func = " \n14"
    Dim Fname As String
    ActiveSheet.Name = "masht"
    'place a data file(.dx) name including drive and
    ' directory in the worksheet Cell "a5".
    Fname = Cells(5, 1)
    Workbooks.OpenText Filename:=Fname, Origin:=xlMSDOS, _
        StartRow:=1, DataType:=xlDelimited, TextQualifier:= _
        xlDoubleQuote, ConsecutiveDelimiter:=True, Tab:=True, Semicolon
        :=False, Comma:=False, Space:=True, Other:=True, OtherChar _
        :="="
End Sub
'
'
'
Sub Macro1()
Attribute Macro1.VB_ProcData.VB_Invoke_Func = " \n14"
    Dim Tite As String
    ActiveSheet.Name = "sht1"
    Range("e10").Select
    ActiveCell.FormulaR1C1 = _
        "=R1C2&"&" "&"&R1C3&"&" "&"&R1C4&"&" "&"&R1C5&"&" "&"&R1C6&"&"
        "&"&R1C7&"&" "&"&R1C8&"&" "&"&R1C9&"&" "&"&R1C10&"&" "&"&R1C11&"&" "&"&R1C12&"&"
        "&"&R1C13&"
    Tite = Cells(10, 5)
    Range("E9").Select
    ActiveCell.FormulaR1C1 = "="&"a17..b"&"&RC[2]"
    Range("G9").Select
    ActiveCell.FormulaR1C1 = "=16+R[5]C[-5]"
    Range("F9").Select
End Sub
'
'
'
'
Sub Macro6()
Attribute Macro6.VB_ProcData.VB_Invoke_Func = " \n14"

```

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APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA (CONT'D)

```

Dim Tite As String
Dim xminz As Single
Dim xmaxz As Single
Dim L As String
Dim ymaxz As Single
ActiveSheet.Name = "sht1"
L = Cells(9, 5)
Tite = Cells(10, 5)
xminz = Cells(12, 2)
xmaxz = Cells(13, 2)
ymaxz = Cells(8, 2)
Charts.Add
ActiveChart.ChartWizard Source:=Sheets("sht1").Range(L), _
    Gallery:=xlXYScatter, Format:=2, PlotBy:=xlColumns, _
    CategoryLabels:=1, SeriesLabels:=0, HasLegend:=2, Title:=
    Tite, CategoryTitle:="WAVELENGTH (NM)", ValueTitle:="OPTICAL
DENSITY", _
    ExtraTitle:=""
ActiveChart.Axes(xlCategory).Select
With Selection.Border
    .ColorIndex = 1
    .Weight = xlHairline
    .LineStyle = xlContinuous
End With
With Selection
    .MajorTickMark = xlOutside
    .MinorTickMark = xlOutside
    .TickLabelPosition = xlNextToAxis
End With
With ActiveChart.Axes(xlCategory)
    .MinimumScale = xminz
    .MaximumScale = xmaxz
    .MajorUnit = 100
    .MinorUnit = 50
    .Crosses = xlCustom
    .CrossesAt = xminz
    .ReversePlotOrder = False
    .ScaleType = False
End With
With Selection.TickLabels.Font
    .Name = "Arial"
    .FontStyle = "Regular"
    .Size = 12
    .Strikethrough = False
    .Superscript = False
    .Subscript = False
    .OutlineFont = False
    .Shadow = False
    .Underline = xlNone
    .ColorIndex = xlAutomatic
    .Background = xlAutomatic
End With

```


APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA (CONT'D)

```
Selection.TickLabels.Orientation = xlHorizontal
ActiveChart.Axes(xlValue).Select
With Selection.Border
    .ColorIndex = 1
    .Weight = xlHairline
    .LineStyle = xlContinuous
End With
With Selection
    .MajorTickMark = xlOutside
    .MinorTickMark = xlOutside
    .TickLabelPosition = xlNextToAxis
End With
With ActiveChart.Axes(xlValue)
    .MinimumScale = 0
    .MaximumScale = ymaxz
    .MinorUnit = 0.1
    .MajorUnit = 0.2
    .Crosses = xlCustom
    .CrossesAt = 0
    .ReversePlotOrder = False
    .ScaleType = False
End With
With Selection.TickLabels.Font
    .Name = "Arial"
    .FontStyle = "Regular"
    .Size = 12
    .Strikethrough = False
    .Superscript = False
    .Subscript = False
    .OutlineFont = False
    .Shadow = False
    .Underline = xlNone
    .ColorIndex = xlAutomatic
    .Background = xlAutomatic
End With
Selection.TickLabels.NumberFormat = "General"
Selection.TickLabels.Orientation = xlUpward
ActiveChart.PlotArea.Select
With Selection.Border
    .ColorIndex = 16
    .Weight = xlThin
    .LineStyle = xlContinuous
End With
Selection.Interior.ColorIndex = xlNone
ActiveChart.Deselect
ActiveChart.SeriesCollection(1).Select
With Selection.Border
    .ColorIndex = 1
    .Weight = xlHairline
    .LineStyle = xlContinuous
End With
```

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APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA (CONT'D)

```

    With Selection
        .MarkerBackgroundColorIndex = 25
        .MarkerForegroundColorIndex = 25
        .MarkerStyle = xlNone
        .Smooth = False
    End With
    ActiveChart.Deselect
End Sub
'
'
'
'
Sub Macro7()
Attribute Macro7.VB_ProcData.VB_Invoke_Func = " \n14"
    ActiveChart.Axes(xlCategory).AxisTitle.Select
    'Selection.Characters.Text = "WAVELENGTH (Start:=1, Length:=8)"
    With Selection.Characters.Font
        .Name = "Arial"
        .FontStyle = "Bold"
        .Size = 12
        .Strikethrough = False
        .Superscript = False
        .Subscript = False
        .OutlineFont = False
        .Shadow = False
        .Underline = xlNone
        .ColorIndex = xlAutomatic
    End With
    ActiveChart.Deselect
End Sub
'
'
'
'
Sub Macro8()
Attribute Macro8.VB_ProcData.VB_Invoke_Func = " \n14"
    ActiveChart.ChartTitle.Select
    With Selection.Font
        .Name = "Arial"
        .FontStyle = "Bold"
        .Size = 12
        .Strikethrough = False
        .Superscript = False
        .Subscript = False
        .OutlineFont = False
        .Shadow = False
        .Underline = xlNone
        .ColorIndex = xlAutomatic
        .Background = xlAutomatic
    End With
    ActiveChart.Deselect
End Sub

```

APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA (CONT'D)

```
'
'
Sub Macro9()
Attribute Macro9.VB_ProcData.VB_Invoke_Func = " \n14"
ActiveChart.Axes(xlValue).AxisTitle.Select
With Selection.Font
    ' For Y axis Title such as O.D.
    .Name = "Arial"
    .FontStyle = "Bold"
    .Size = 12
    .Strikethrough = False
    .Superscript = False
    .Subscript = False
    .OutlineFont = False
    .Shadow = False
    .Underline = xlNone
    .ColorIndex = xlAutomatic
    .Background = xlAutomatic
End With
ActiveChart.Deselect
End Sub
'
'
Sub Macro10()
Attribute Macro10.VB_ProcData.VB_Invoke_Func = " \n14"
With ActiveChart.PageSetup
    .LeftHeader = ""
    .CenterHeader = ""
    .RightHeader = ""
    .LeftFooter = ""
    .CenterFooter = ""
    .RightFooter = ""
    .LeftMargin = Application.InchesToPoints(1.5)
    .RightMargin = Application.InchesToPoints(0.5)
    .TopMargin = Application.InchesToPoints(0.75)
    .BottomMargin = Application.InchesToPoints(1.25)
    .HeaderMargin = Application.InchesToPoints(0)
    .FooterMargin = Application.InchesToPoints(0)
    .ChartSize = xlFullPage
    .PrintQuality = 300
    .CenterHorizontally = False
    .CenterVertically = False
    .Orientation = xlLandscape
    .Draft = False
    .PaperSize = xlPaperLetter
    .FirstPageNumber = xlAutomatic
    .BlackAndWhite = False
    .Zoom = 100
ActiveChart.Deselect
End With
End Sub
```

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APPENDIX C. MACRO FOR PLOTTING ABSORPTION SPECTRA (CONT'D)

```
Sub Macro11()  
Attribute Macro11.VB_ProcData.VB_Invoke_Func = " \n14"  
ActiveChart.PlotArea.Select  
    Selection.Height = 450  
    Selection.Top = 0  
    Selection.Width = 541  
ActiveChart.Deselect  
    'height 450 and width 541 gives 3to4 ratio in the plot proper. Font  
size etc may change this ratio. Watch for the "page setup " too.  
    '.LeftMargin = Application.InchesToPoints(1.5)  
    '.RightMargin = Application.InchesToPoints(0.5)  
    '.TopMargin = Application.InchesToPoints(0.75)  
    '.BottomMargin = Application.InchesToPoints(1.25)  
    '.HeaderMargin = Application.InchesToPoints(0)  
    '.FooterMargin = Application.InchesToPoints(0)  
End Sub
```

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