

Structural Identification of Prosthetics/Orthotics Polymers Using Infrared Spectral Searching

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SYNOPSIS

The suitability of a combination of an infrared spectral search program and three commercially available infrared spectral data bases to structurally identify prosthetics/orthotics polymers was assessed. Five currently used prosthetics/orthotics polymers subjected to a simulated clinical fabrication heat treatment were examined using diffuse reflectance. The polymers selected were Durr-Plex (polyethylene terephthalate), polypropylene, Subortholen (polyethylene), Surlyn (ethylene methacrylate ionomer), and Uvex (cellulose acetate butyrate). The combination of a spectral search program and three commercially available data bases was inadequate for structural identification of these prosthetics/orthotics polymers in their simulated clinical fabrication heat-treated condition and may be misleading. Benefits of creating effective combinations of spectral search software and appropriate and more comprehensive data bases with specific entries for prosthetics/orthotics polymers would be for: (1) quality control of batches of polymers, and (2) the development of standards, test methods necessary to evaluate the effects of environmental influences associated with long-term clinical service. © 1996 John Wiley & Sons, Inc.

INTRODUCTION

Prosthetic and orthotic devices are needed with optimal physical and mechanical properties over the range of clinical activities and life-span. Therefore, the structural characterization and the influence of structure on the physical and mechanical properties are essential to that goal of optimization. A systems approach for improvement in prosthetic and orthotic devices advocated by White,¹ incorporating input from medical, engineering, and materials sciences, may be a more valuable route than uncoordinated efforts to optimize the final product for physical and mechanical properties.

As a result of concern in the international community about the need to provide prostheses that were safe for use by amputees, and also because

of an awareness that test standards would assist the development of better prostheses, the International Organization for Standardization (ISO) Technical Committee 168 has continued work leading to the development of the international standard, ISO 10328, Prosthetics-Structural Testing of Lower Limb Prostheses.² The Committee has recognized the limitations of this standard and identified directions that should be undertaken. Ideally, additional laboratory tests dealing with function, wear and tear, and environmental influences should be carried out as part of the evaluation procedure. There are no standards for such tests, so appropriate procedures will need to be specified.²

In an effort to develop analytic tools for the study of prosthetics/orthotics polymers, it was of interest to determine if infrared spectral searching of commercially available data bases could be employed for structural identification. This structural identification could become important for quality control, failure analysis, and correlation with clinical outcomes.

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Fourier transform infrared (FTIR) spectroscopy can be used to determine structures because certain aggregates of atoms (functional groups) can be associated with definite characteristic absorption bands. The absorption of infrared radiation occurs over certain frequency intervals. The infrared spectrum of any given substance is interpreted by the use of these known group frequencies to characterize the substance as one containing a given type of group or groups. Functional groups sometimes have more than one characteristic absorption band associated with them. Two or more functional groups may absorb in the same region and can only be distinguished from each other by means of other characteristic infrared bands that occur in nonoverlapping regions.^{3,4} Infrared group frequencies are only applicable for specific spectra structure identification when the infrared spectrum of the unknown polymer is recorded in the same manner as that used to record the infrared spectra used to build the infrared group-frequency data base.⁵

Systems have been developed to handle varying quantities of data and allow for archiving, accessing, and analysis.⁶⁻¹⁰ Quality criteria have been established for digital infrared reference spectra.¹¹ Desirable search performance methods need high discrimination ability and resistance to peak height variation and peak position shifts due to experimental conditions such as concentration and noise.¹²⁻¹⁵

Computerized data bases developed to optimize polymer selections have been described.¹⁶ Unique infrared spectral data bases have been developed for several specialized techniques: infrared microspectroscopy of fibers¹⁷ and infrared vapor-phase libraries for matrix isolation spectral searching.¹⁸ Searching software and data bases may be obtained from the same manufacturer as for the infrared spectroscopy instrumentation, other infrared manufacturers, or from noninstrumentation companies. For example, a software company, Galactic Industries (Salem, NH), and a division of an instrumentation manufacturer, Sadtler, (Division of Bio-Rad, Philadelphia, PA), both offer search software that can use spectral data files in the JCAMP-DX format created on many instrumentation systems. The JCAMP-DX standard is an adaption of software written by Dr. Robert McDonald¹⁹ under contract to the Committee on Spectral Portability working under the auspices of the Joint Committee on Atomic and Molecular Physical Data and provides a means for transferring spectral data between dissimilar systems. Typical of instrument manufacturers, Nicolet (a subsidiary of Thermo Instrument

Systems Inc., a Thermo Electron company, Madison, WI), lists 30 spectral data bases to cover various types of materials and conditions of testing. In addition, there are Aldrich and Sigma Condensed Phase data base subsets available to focus on particular chemical groups or biologically related materials and more than 50 data base collections from Sadtler.

A common graphical user interface and spectral search software and data bases purchased from the same company may contribute to ease of usage and familiarity. There has been a trend for IBM[®]-compatible computers to utilize the Windows[™] software as a common graphical user interface. Recently, a spectral identification software package that was a Windows-based application has been reviewed.²⁰ Because there are no industry standards for how software packages should perform, it is not clear about the suitable combinations for prosthetics/orthotics applications that would allow for effective identification of classes of materials and specific functional groups.

This investigation evaluated a combination of a spectral search program and three commercially available infrared spectroscopic data bases for their suitability in the structural identification of simulated clinical fabrication heat-treated prosthetics/orthotics polymers. The spectral search program and the three data bases selected were from the instrumentation manufacturer. Currently used prosthetics/orthotics polymers are frequently heat treated to allow molding around a plaster cast. Thermoforming is considered to be one of the oldest plastics processing techniques.²¹ Investigating prosthetics/orthotics polymers in a simulated clinical fabrication heat-treatment condition could serve as a baseline before subjecting them to clinical service or accelerated weathering conditions. The prosthetics/orthotics polymers were not investigated in the as-received condition.

MATERIALS

The following polymers were investigated: Durr-Plex (DP), Polypropylene (PP), Subortholen (SB), Surlyn (SR), and Uvex (UX). The PP polymer was purchased from Durr-Fillauer Medical, Inc., Chattanooga, TN. The DP, SB, SR, and UX polymers were purchased from PEL Supply Co., Cleveland, OH. The suppliers list the DP, PP, SB, SR, and UX polymers, as being polyethylene terephthalate, polypropylene, polyethylene, ethylene methacrylate ionomer, and cellulose acetate, respectively.

METHODS

Simulated Clinical Fabrication Heat Treatment (SC)

The simulated clinical fabrication heat treatment (SC) method consisted of placing the three polymers, 6" square specimens approximately = 2" thick, on preheated Teflon[®]-coated aluminum sheets in convection-blower ovens (Grieve, Models AB-500 and 3-3-3, Round Lake, IL), heated at the supplier's recommended temperatures for 15–20 min, until bubbles started to form around the periphery, the corners were pliable, and the polymers became transparent. The polymers were then covered with a second, preheated, Teflon[®]-coated aluminum sheet, and allowed to air cool on the bench top. This method of oven heating and air cooling reflects only a part of the current processing of the polymers. The complete sequence for a "clinical fabrication process" would be: convection oven heating, deforming or molding specimens around curved surfaces on cold and often wet plaster casts, and letting the specimens to air cool to room temperature. The use of aluminum sheets allows for a more uniform cooling than cold and/or wet plaster casts. The forming temperatures were 148–163°C for the DP, 204°C for the PP, 177–204°C for the SB, 177°C for the SR, and 148–163°C for the UX polymers, respectively.

Fourier Transform Infrared Spectroscopy

The samples were pulverized in a laboratory mill (W. B. Laboratory Mill, Model S-500, Weber Bros. & White Metal Works, Inc. Hamilton, MI) and cooled with liquid nitrogen to prevent heating of the samples by the rotating knife blades. A KVB Analect model RFX-65 FTIR spectrometer (KVB Analect, Division of Air & Water Technologies, Irvine, CA), with a narrow-band Mercury Cadmium Telluride (MCT) detector, was used for the diffuse reflectance (DR) technique at 4 cm⁻¹ resolution. The DR technique consisted of mixing the samples with KBr powder to an approximate sample concentration from 1 to 5% by weight, and ball-milling the mixture to a fine powder, then focussing the infrared beam on the sample.^{22–24} The amount of the beam that is diffusely reflected through the sample is collected by the detector.

A common technique is the KBr direct transmission disk (DT) technique. For this technique of making a KBr disk, 2–5 mg of the polymer powder are mixed with approximately 80 mg of KBr, hy-

draulically pressed into a disk, and the disk is inserted directly into the path of the infrared beam.²⁵ The amount of the beam that passes through the sample is collected by the detector. As a result of these techniques, interferograms are created that are unique to the polymers. Comparisons have been made between both DR and DT techniques.²⁶ Only one specimen was made of each polymer, as is typical for data bases. Sadtler, which has developed standard techniques in its laboratories to ensure that its published spectra exhibit the highest quality and reproducibility for comparison and identification purposes, notes that each spectrum is labeled with the sample preparation technique used and when applicable, the mass of the sample located in the optical path of the spectrometer at the time the spectrum was recorded.²⁷

SPECTRAL DATA BASE SEARCHING (SDS)

Ideally, the identity of an unknown material should be easily obtained through searching of an appropriate computerized materials data base. Falling short of complete identification for a material directly from an infrared data base, functional group or other structural information to categorize the structure further should be obtained.²⁸

The searching software, HAVEC II[®] (KVB Analect), offers choices of Euclidean distance (ED), absolute difference, derivative absolute difference, and derivative least squares search algorithms. The ED algorithm (Alan Hanna, U.S. Coast Guard, R & D Center, Groton, CT) was used to calculate differences between interferogram segments from a sample and stored data base spectra. The 10 best matches were those spectra displaying the smallest ED from zero. Zero is a complete match. The smaller the distance, the closer the match between the data base spectrum and the spectrum of the unknown material. The distances are relative comparisons. A "good" match ideally has these criteria: it appears in the data base, is feasible, has a low number score, and is recognizable visually.²⁹ A score of 0.100 is a four times better fit than a score of 0.400. A score of 0.001 is very close and has been obtained when reusing the same sample that was used in creating the spectral data base.²⁹ The ED algorithm choice was selected based on an application profile, AP-104 (KVB Analect), which demonstrated identification of a three-component mixture. A correlation search algorithm may be suitable for correctly identifying some polymers such as 2-bromopropane.³⁰ In the correlation search algorithm the first derivative

of the unknown spectrum is correlated with the derivatives of the library spectra. An overall correlation index ranging from 0-100 is calculated.³⁰

Each sample's spectrum was compared to entries in three data bases: polymer, polymer chemical, and fiber (KVB Analect). The combined search listed rankings from the 10 closest matches.

RESULTS

Figure 1, with a unique structural fingerprint pattern for the SB polymer using the DR sample handling technique, is representative of the type of infrared spectra seen for prosthetics-orthotics polymers. It is this spectral uniqueness that is the basis on which the searches were conducted. Peak assignments were made through comparisons with standard infrared tables^{3,31} and are shown in Table I. A complete set of figures showing the infrared spectra for the five polymers: DP, PP, SB, SR, and UX, using two techniques—DR and DT—has previously been reported.²⁶ The top three and appropriate listings in the ranking are given in Table II for the DR technique.

DISCUSSION

Infrared spectral searching of three commercially available data bases, as an analytic tool, was able to provide information regarding the structural characterization of prosthetics/orthotics polymers. It could be a part of a system's approach to laboratory tests dealing with the evaluation of function, wear

Table I Subortholen (SB) Polymer Peak Positions and Assignments

	SC Condition and DR Technique	
	Position	Assignments
A	1176.36	C—C skeletal stretch
B	1305.57	C—H twisting
C	1351.86	C—H deformation
D	1473.35	CH ₂ bending
E	1601.65	C=C stretch
F	1741.41	C=O stretch
G	1897.61	=C—H overtone
H	2632.36	aldehydic C—H stretch
I	2850.27	CH ₂ stretch symmetric
J	2917.77	CH ₃ stretch asymmetric
K	3370.96	O—H stretch

and tear, and environmental influences, and may address some of the recognized limitations and identified directions that should be undertaken as suggested in the test standard, ISO 10328, Prosthetics-Structural Testing of Lower Limb Prostheses.² Problems and limitations of the spectral search software data bases combination were noted in the areas of appropriate entries, infrared technique, the ED between the entries, and sample condition considerations.

In the rank listings for the polyethylene polymer, SB, there should be entries of polyethylene, or entries of polyethylene as a part of the polymer selected, based on the observation that similar polymers structurally, produce similar spectra. The results for the SB polymer had several polyethylene listings, but based on the numerous polyethylene

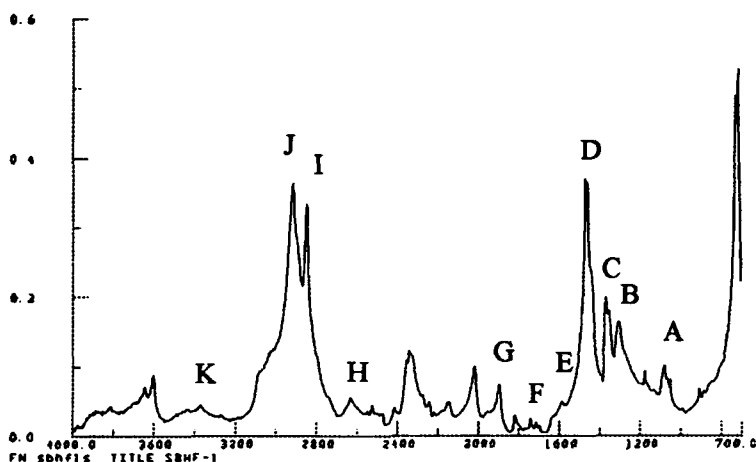


Figure 1 Infrared spectrum of the subortholen polymer (SB) using the diffuse reflectance technique.

Table II Spectral Data Base Rankings, DR Technique**Polymer: Durr-Plex (DP)**

Rank	E.D.	data base index name
1.	.073	cellulose acetate butyrate
2.	.086	acetyl tributyl citrate
3.	.093	cellulose proprionate

Polymer: Polypropylene (PP)

Rank	E.D.	data base index name
1.	.087	Chevron Chemical POLYLOOM [®] , olefin
2.	.091	Chevron Chemical POLYLOOM [®] , olefin, different fiber (unspecified)
3.	.104	polypropylene, amorphous

Polymer: Subortholen (SB)

Rank	E.D.	data base index name
1.	.098	<i>n</i> -ocatadecane
2.	.118	tristearyl citrate
3.	.119	octadecyl-3,5-di- <i>t</i> -butyl-4-hydroxycinnamate
7.	.123	Kodak EPOLENE [®] C-13 polyethylene
10.	.127	Phillips MARLEX [®] polyethylene

Polymer: Surlyn (SR)

Rank	E.D.	data base index name
1.	.079	2-methoxyethyl stearate
2.	.087	<i>n</i> -octacecane
3.	.094	rosin oil high viscosity
4.	.094	Allied polyethylene & copolymer

Polymer: Uvex (UX)

Rank	E.D.	data base index name
1.	.052	Hoechst Fibers TREVIRA [®] polyester fiber 52
2.	.052	E.I. du Pont DACRON [®] polyester fiber 27
3.	.053	E.I. du Pont DACRON [®] polyester fiber 21
4.	.053	Hoechst Fibers TREVIRA [®] polyester fiber 53
5.	.054	Hoechst Fibers TREVIRA [®] polyester fiber 46
6.	.054	Eastman Chemical KODEL [®] polyester
7.	.054	Allied Chemical polyester
8.	.054	Enke polyester
9.	.055	E.I. du Pont DACRON [®] polyester
10.	.055	Avtex Fibers AVLIN [®] polyester

entries in the data base, only polyethylene-related entries would be expected. The DP polymer search indicated an ester structure but did not indicate the presence of the ethylene or phthalate structure. The PP polymer search indicated amorphous polypropylene and polymers with propyl groups, but did not list isotactic polypropylene. For the SR polymer, polyethylene was listed with a copolymer but not as a separate entry.

The spectral search results listed in this article were created with the DR sampling technique.

Spectra had been created with both DR and DT sampling techniques as a methods comparison.²⁶ The DR and DT techniques may not give identical results due to the differences in the physical processes that occur for the transmission and diffuse reflectance techniques. In KBr disk transmission sampling, DT, all of the transmitted radiation traverses the same pathlength. In KBr diffuse reflectance, DR, a number of different individual pathlengths are possible, because the interaction of the beam with the polymer results in a combination of reflected and transmitted

wavelengths. The average pathlengths experienced by strongly absorbed wavelengths, would be expected to be quite small. Even for strongly absorbed wavelengths some radiation will be diffusely reflected, as they will have penetrated only a short distance through the sample before being backscattered to the surface. The weakly absorbed wavelengths may penetrate quite deeply into the sample, effectively sampling a much greater amount of polymer. As such, these wavelengths will be absorbed much more than might be expected, enhancing the spectra. The enhancement in the lower wavenumber region was evident as compared to the weaker absorptions seen in transmittance sampling and may be advantageous in discriminating between spectra if the spectral data base had entries that were created with the DR technique. The spectra from polymers using the DT technique had broader peaks at 3600–3200 and 1800–1500 cm^{-1} , whereas the spectra using the DR technique had an accentuated 1400–800 cm^{-1} region.²⁶ The DR technique E.D. values and ranges were: for the DP polymer, 0.073–0.111 (0.038); for the PP polymer, 0.087–0.129 (0.042); for the SB polymer, 0.098–0.127 (0.029); for the SR polymer, 0.079–0.105 (0.026); and for the UX polymer, 0.052–0.055 (0.003). The E.D. for the UX polymer had a 0.0–0.002 difference between entries. This phenomena of small E.D. values and close ranges was similar to that seen in the DT technique. The DT technique E.D. values and ranges were: for the DP polymer, 0.127–0.136 (0.009); for the PP polymer, 0.127–0.145 (0.018); for the SB polymer, 0.081–0.110 (0.029); for the SR polymer, 0.085–0.114 (0.029); and for the UX polymer, 0.108–0.114 (0.006).^{30,31} These small E.D. differences may not allow for adequate discrimination.

Measurements of consistency among different specimens of the same polymer for infrared spectroscopic examination may be considered from data used for degree of conversion of the $\text{C}=\text{C}$ to $\text{C}-\text{C}$ bonds in polymers. Using $\text{C}=\text{O}$, $\text{O}-\text{H}$, and $\text{N}-\text{H}$ peaks in a peak height ratioing technique, the standard deviations ranged from 2.6–11.8% of the calculated degree of conversion, depending on the peaks selected.³² Because noise has been shown to detrimentally influence the success of spectral searching,³⁰ variation in peak heights may also influence the search calculations. An application program, RAZOR[™] (Spectrum Square Associates, Inc., Ithaca, NY), offers three methods to remove noise from a spectrum. Further studies with noise removal methods are indicated.

Most search processes work best with pure compounds.¹² All but the SR polymer were ho-

mopolymers (composed of only one type of polymer). The UX search rank listing had 10 polyester entries similar to each other, but no entry for cellulose acetate butyrate from the Polymer data base even though it was a possibility for that data base. This may be related to differences in the methods of preparation for the polymers and/or sampling techniques.

Most of the entries selected using the Polymer and Fiber data bases were not included in a standard reference book: The Desk-Top Data Bank[™].³³ For entries with tradenames, associating the generic/chemical names, exact composition, and manufacturer, would be helpful to know. KVB Analect did not always list the sample preparation methods used for the polymers in these data bases. In other data bases, such as the Georgia State Crime Lab (KVB Analect) and the Canadian Forensics (KVB Analect) data bases, some information about sample condition or preparation was given and the particular spectroscopic technique used was implied.

When the DT disk technique spectrum for each polymer was incorporated into the Polymer data base and a search performed, the search algorithm matched the polymers as the number 1 ranking with an E.D. of 0.000.²⁶ Inclusion of data bases with inappropriate entries into the search may produce incorrect match entries as seen for the SB polymer, entry #2, tristearyl citrate and no listing of polyethylene or polyethylene terephthalate in the ranking for the DP polymer. The justification for the combination of the data bases was that entries do exist within the combination to allow for matching of most of the prosthetics/orthotics polymers. The Polymer data base contained isotactic polypropylene, cellulose acetate, cellulose acetate butyrate, poly diallyl phthalate, polyethylmethacrylate, and ethylene/acrylic acid copolymer (20% acrylic acid), and several polyethylene spectra. The Fibers data base contains Dacron[™] (polyethylene terephthalate).

Because newly created spectra were added to the Polymer data base using the written instructions provided by KVB Analect in order to validate the E.D. mathematical procedure,²⁶ feasibility of the creation of comprehensive spectral data bases of common prosthetics/orthotics polymers was demonstrated. Regarding data base modification, spectra can be added to any of the existing KVB Analect data bases or ones developed by the user. The acquisition of the spectra for inclusion into data bases was the same as for any other situation.²⁶ There were no changes in instrument op-

erator skills or additional cost. Spectra can be imported to other software programs such as GRAMS/386™ (Galactic Industries), which have spectral searching capabilities.

When a peak of interest is highlighted in a window, the IR Mentor™ and Interpret IR™ software packages can locate and display functional groups with characteristic bands at that frequency. While not specifically identifying polymers, identifying the components may contribute to the recognition of polymers. These software packages may be valuable for the purpose of identifying the functional groups.³⁴

These polymers were in the SC condition, in part, to simulate the condition of currently used polymers. Investigating polymers in the simulated clinical fabrication heat-treatment condition could serve as a baseline before subjecting them to clinical service or accelerated weathering conditions such as exposure to ultraviolet light and heated condensation and then monitoring the degradation changes. Because computer-aided design/computer-aided manufacturing (CAD-CAM) systems (System Shape™, University College London, London, UK) can use polymers in the as-received condition, polymers should be investigated in this condition also. Infrared spectral searching methods would be complementary to other techniques such as nuclear magnetic resonance spectroscopy³⁵ and x-ray diffraction³⁶ for structure identification.

The problems and limitations with the commercially available data bases may be the following: (1) appropriate number of matches due to data base composition, particularly the presence or absence of the exact polymer; (2) spectral differences due to sample preparations or spectroscopic techniques; and (3) inadequate information given by the software vendor regarding the polymers' composition and spectroscopic technique for the data base. In terms of the combination of the spectral search software and data bases, the problems and limitations may be a function of: (1) the spectral search software, (2) the data bases, or (3) the combination of the the searching software and the data bases. Further investigation to address these concerns would consist of: (1) testing software from different companies using the various search choices but the same data bases, and (2) testing the same searching software from a given company with different data bases containing the same entries but modified sample preparations. Then an assessment should be made of the variations in mismatch due to the relative contributions of the searching software and the data bases.

CONCLUSIONS

The combination of a spectral search software program and three data bases investigated was shown to be inadequate for structural identification of five prosthetics/orthotics polymers, and may yield misleading results. Combinations of software and the data bases with proper entries for prosthetics/orthotics polymers need to be created for effective structural identification. Each entry should contain the tradename, generic/chemical name, composition, manufacturer, condition of sample, and sampling technique. This information should be easily accessible to the user.

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