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ESTIMATION OF ORGANIC AND INORGANIC MATTER IN INLAND WATERS: OPTICAL CROSS SECTIONS OF LAKES ONTARIO AND LADOGA

R.P. Bukata, J.H. Jerome, K. Ya. Kondratyev and D.V. Pozdnyakov

NWRI CONTRIBUTION 90-166

RRB 90-65

ESTIMATION OF ORGANIC AND INORGANIC MATTER IN INLAND WATERS: OPTICAL CROSS SECTIONS OF LAKES ONTARIO AND LADOGA

by

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MANAGEMENT PERSPECTIVE

This work represents the initial, in what is hoped to be a series, of collaborations between the Rivers Research Branch of NWRI and the Institute for Lakes Research of the USSR Academy of Sciences. An optical model, developed by the NWRI Spectro-Optics Group and designed to remotely estimate simultaneous concentrations of chlorophyll, suspended sediments, and dissolved organic matter from optically-complex inland waters, has been applied by Soviet scientists to the remote sensing of Russian waters. Excellent agreement (and therefore model verification) has been obtained between such optical modelling and monitoring in Lake Ontario and Lake Ladoga.

PERSPECTIVE GESTION

Le présent travail représente le premier d'une série de travaux de collaboration, espérons-le, entre le Direction de la recherche sur les cours d'eau de l'INRE et l'Institut de recherche sur les cours d'eau de l'Académie des sciences de l'URSS. Un modèle optique, élaboré par le groupe de la spectro-optique de l'INRE et conçu pour évaluer à distance des concentrations simultanées de chlorophylle, de sédiments en suspension et de matières organiques dissoutes des eaux intérieures optiquement complexes, a été appliqué par des scientifiques soviétiques pour la télédétection des eaux en Russie. Une concordance excellente (et par conséquent la vérification du modèle) a été obtenue entre ce genre de modélisation et de surveillance optiques dans le lac Ontario et le lac Ladoga.

ABSTRACT

The high degree of optical complexity of inland water masses necessitates the development of models which consider the optical competitiveness of several co-existing aquatic components. A model is described which was developed to simultaneously extract chlorophyll a, suspended mineral, and dissolved organic carbon concentrations from a single measurement of the subsurface volume reflectance spectrum in the optically complex waters of Lake Ontario. To extract such aquatic concentrations requires a quantification, as a function of wavelength, of the amount of scattering and absorption that may be ascribed to a unit concentration of each aquatic component (i.e. the pertinent optical cross sections). Cross section spectra are presented for Lake Ontario and it is illustrated how such cross sections may be utilized in conjunction with directly-measured subsurface volume reflectance spectra and optimization analyses to extract the organic and inorganic components. Cross section spectra obtained in a similar manner for Lake Ladoga are also presented and compared to those of Lake Ontario.

RÉSUMÉ

Le niveau élevé de complexité optique des masses d'eau intérieures exige le développement de modèles qui tiennent compte de la compétitivité optique de plusieurs composantes aquatiques coexistantes. On décrit un modèle qui a été élaboré afin d'extraire simultanément les concentrations de chlorophylle a, de minéraux en suspension et de carbone organique dissous à partir d'une seule mesure du spectre de réflectance volumique sous la surface des eaux optiquement complexes du lac Ontario. Pour obtenir ces concentrations aquatiques, il faut mesurer, en fonction de la longueur d'onde, la proportion d'onde de dispersion et d'absorption qui peut être attribuée à une unité de concentration de chacune des composantes aquatiques (c'est-à-dire les vues optiques pertinentes en coupe). On présente des spectres de vues en coupe du lac Ontario, et on montre comment des vues en coupe peuvent être utilisées conjointement avec des spectres de réflectance volumique sous la surface de l'eau mesurés directement et des analyses d'optimisation pour extraire les composantes organiques et inorganiques. Des spectres des vues en coupe obtenus de la même manière dans le cas du lac Ladoga sont également présentés et comparés à ceux du lac Ontario.

INTRODUCTION

It is well known that the combined processes of scattering and absorption dictate the manner in which impinging radiation propagates through a natural water mass. Since each water mass is comprised of a specific combination of organic and inorganic scattering and absorption centres, the energy spectrum returning both to and through the air-water interface subsequent to volumetric interactions, will be characterized by a spectral signature pertinent to the composition of the water mass under consideration at that particular time and location.

The direct linkages between upwelling energy spectra and the components of a natural water mass are the optical cross sections of these aquatic components, i.e. the quantification of the scattering and absorption that may be ascribed to a unit concentration of each aquatic component. Such optical cross sections are clearly dependent upon not only the physical and biological characteristics of the aquatic components, but also upon the wavelength of the impinging radiation.

It is the purpose of this communication to review modelling activity performed at The National Water Research Institute to obtain such optical cross sections for Great Lakes waters. Spectra of scattering and absorption cross sections obtained in Lake Ontario will be compared to cross section spectra obtained in Lake Ladoga by The Institute for Lakes Research in Leningrad.

The objective of the optical modelling was to develop a technique by which simultaneous estimates of organic and inorganic concentrations could be obtained from a single optical measurement in

inland waters. Such a technique will be briefly described and data from Lake Ontario will be presented to illustrate its application.

It is the purpose of our companion paper (Bukata et al., 1991) to illustrate the role of such a model in the remote estimation of aquatic productivity, and to strongly advocate the incorporation of remote monitoring of lake chlorophyll (through the use of appropriate cross sections) into the global climate change studies of the upcoming decades.

MODELLING THE OPTICALLY-COMPETITIVE NATURE OF INLAND WATERS

Studies of the optical properties of natural waters must contend with two broad categories of optical properties. The apparent optical properties of a water mass are those that are dependent upon the spatial distribution of the impinging radiation. The inherent optical properties of a water mass are those that are totally independent of the spatial distribution of the impinging radiation.

One readily-measurable apparent optical property is the subsurface volume reflectance (irradiance reflectance), $R(\lambda)$, which may be obtained from <u>in situ</u> determinations of the upwelling and downwelling irradiance spectra utilizing submersible spectroradiometers. Also, readily obtained from spectrometric measurements is the apparent optical property irradiance attenuation coefficient $k(\lambda)$.

The inherent optical properties of a water mass include the total attenuation coefficient $c(\lambda)$, the absorption coefficient $a(\lambda)$, the scattering albedo $\omega_0(\lambda)$, the scattering coefficient $b(\lambda)$, the forwardscattering probability $F(\lambda)$, the backscattering probability

$B(\lambda)$, and the volume scattering function $\beta(\theta)$. With the exception of $c(\lambda)$ which is determined from transmissometry, the inherent optical properties are not readily-measurable parameters. Such inherent optical properties have come to be traditionally inferred from directly-measurable apparent optical properties. This is accomplished by means of suitable representations of the radiative transfer equation such as those utilized in the models of Gordon et al. (1975), DiToro (1978) and Kirk (1984).

In the current work we have utilized a Monte Carlo simulation of photon propagation to determine the relationships among the volume reflectance just beneath the air-water interface, the absorption coefficient a, and the backscattering coefficient Bb. This Monte Carlo simulation was employed for both ocean and lake waters as detailed in Jerome et al. (1988).

Elsewhere (Bukata et al., 1985; Kondratyev and Pozdnyakov, 1988) we have detailed the methodologies by which direct measurements of subsurface volume reflectance R, irradiance attenuation coefficient k, and the total attenuation coefficient c (all as functions of wavelength λ and depth z) may be used to infer concentrations of chlorophyll a, suspended minerals (i.e. suspended sediments), and dissolved organic carbon (i.e. yellow substances). Such work, performed in the optically complex waters of Lake Ontario in North America and Lake Ladoga in Northern Europe, resulted from coordinated efforts of optical and water quality data collection, multiple regression, radiative transfer theory and optimization analyses which interwove in the manner schematically illustrated in the flow diagram of Figure 1. Directly-measured *in situ* optical parameters $R(\lambda)$, $k(\lambda)$, and $c(\lambda)$ are relatable through radiative transfer equations to the

inherent optical properties $a(\lambda)$, $b(\lambda)$ and $B(\lambda)$. These inherent optical properties are a direct consequence of the individual optical properties of each of the organic and inorganic, suspended and dissolved, scattering and absorption centres comprising the water mass under consideration. Our optical water quality model restricted itself to three broad component categories and considered the scattering and absorption properties of chlorophyll a (uncorrected for phaeophytin contamination), suspended minerals (irrespective of type) and dissolved organic carbon, as well as pure water itself. The inherent optical properties display additive properties. Thus, for each wavelength λ, these additive properties may be mathematically expressed as:

$$a = \sum_{i=1}^{n} x_i a_i \tag{1}$$

$$b = \sum_{i=1}^{n} x_i b_i \tag{2}$$

$$Bb \equiv \sum_{i=1}^{n} x_i B_i b_i \tag{3}$$

where $x_i \equiv$ concentration of the ith component of the water mass

$a_i \equiv$ absorption coefficient at wavelength λ for a unit concentration of component i

$b_i \equiv$ scattering coefficient at wavelength λ for a unit concentration of component i.

$B_i b_i \equiv$ backscattering coefficient at wavelength λ for a unit concentration of component i.

The optical cross sections a_i, b_i and $B_i b_i$ are the direct links between the inherent optical properties of a water mass and its optically-active components. As shown in Figure 1, these optical cross sections may be determined by utilizing multiple regression or optimization analyses. One significant advantage of using optimization analyses (Bukata et al. 1985) is the fact that the essential cross sections a_i and $B_i b_i$, may be determined solely from subsurface volume reflectance $R(\lambda)$ and concentrations of the optically-active aquatic components.

Once the wavelength-dependent optical cross sections are known, a theoretically-anticipated volume reflectance spectrum $R(\lambda)$ may be generated for any pre-selected combination of chlorophyll (Chl a), suspended mineral (SM), and dissolved organic carbon (DOC) concentrations (the three principal components of our water quality model).

As described in Jerome et al. (1988), the results of the Monte Carlo simulation relating volume reflectance $R(\lambda)$ just beneath the air-water interface to the inherent optical properties a and Bb yield the equations

$$R = 0.319 \frac{Bb}{a} \tag{4}$$

for $0 \leq \frac{Bb}{a} \leq 0.25$ and

$$R = 0.267 \frac{Bb}{a} + 0.013 \tag{5}$$

for $0.25 \leq \frac{Bb}{a} \leq 0.50$

Equations (4) and (5) apply to each wavelength within the considered optical spectrum.

Using optimization analyses, directly-measured (or remotely-inferred) volume reflectance spectra may then be fitted with theoretically predicted spectra from equations (4) and (5). Such optimization is accomplished by simultaenously varying the concentrations of chlorophyll, suspended minerals, and DOC. Multivariate optimization techniques such as the Levenberg-Marquardt finite difference algorithms (Levenberg, 1944; Marquardt, 1963) are required for the extraction of water quality information from such volume reflectance spectra.

OPTICAL CROSS SECTIONS OF LAKE ONTARIO

Following Bukata et al. (1983; 1985), the optical cross sections (for suspended minerals, chlorophyll a uncorrected for phaeophytin, and dissolved organic carbon) determined for Lake Ontario are shown in Figures 2 and 3 as well as the corresponding attenuation coefficients of pure water. Figure 2 illustrates the absorption cross sections as a function of wavelength, while Figure 3 illustrates the scattering cross sections as a function of wavelength. The scattering cross section of dissolved organic carbon is taken to be zero at every wavelength.

Figure 4 illustrates a representative sample of directly-measured volume reflectance spectra (obtained by the National Water Research Institute using a Techtum QSM 2500 scanning Quantaspectrometer) observed at both nearshore and midlake stations visited during May, July, and September, 1979. Although the actual magnitudes of the

observed volume reflectances may vary (a direct consequence of the spatial and temporal variabilities of the optically-active concentrations) a pronounced peak at mid-wavelengths is a recognizable feature of each optical spectrum. This is a consequence of the fact (as seen from Figures 2 and 3) that the optical cross sections of chlorophyll a, suspended minerals, and dissolved organic carbon are such that all three components reduce the relative volume reflectance values at lower values of λ (compared to mid wavelength values) as the concentrations of the components increase.

Figure 5 depicts an example of the simultaneous extraction of concentrations of chlorophyll a, suspended minerals, and dissolved organic carbon from an *in situ* Lake Ontario volume reflectance spectrum utilizing the optical water quality model. Herein is shown the comparison between the calculated "best fit" and the directly-measured volume reflectance spectra for a Niagara River plume station in western Lake Ontario. The "best fit" curve (solid circles, joined points) was calculated utilizing the Levenberg-Marquardt multivariate optimization technique along with the absorption and scattering cross section spectra of Figures 2 and 3. The predicted values of chlorophyll a, suspended mineral, and dissolved organic carbon concentrations required to generate the "best fit" optical spectrum are listed in Figure 5. Also listed are the concentrations obtained from water samples collected at the time of the optical observations. It is seen that the optical water quality model can predict acceptable values of simultaneous concentrations of chlorophyll a, suspended minerals, and dissolved organic carbon from a single spectral measurement of subsurface volume reflectance once the optical cross sections are known.

OPTICAL CROSS SECTIONS OF LAKE LADOGA

During the 1988 and 1989 field seasons, the Institute for Lakes Research of the USSR Academy of Sciences conducted coordinated studies of Lake Ladoga in Northern Europe. In a manner similar to the study performed in Lake Ontario a decade earlier, subsurface volume reflectance spectra were measured simultaneously with the collection of water samples to determine concentrations of suspended minerals, chlorophyll, and dissolved organic carbon. Radiative transfer theory and optimization analyses were then employed (as shown in Figure 1) to obtain the optical cross sections appropriate to Lake Ladoga.

Figure 6 illustrates the absorption cross section spectrum obtained for the suspended mineral component of Lake Ladoga in 1988 and 1989. Also shown is the suspended mineral absorption cross section spectrum obtained in Lake Ontario a decade earlier. Figure 7 illustrates a similar Lake Ladoga/Lake Ontario comparison for the respective backscattering cross section spectra of indigenous suspended minerals. Since the scattering and absorption of suspended minerals are directly dependent upon particle size, shape and refractive index, the geology of an inland water's drainage basin will directly dictate the optical cross sections of suspended minerals indigenous to the aquatic regime. Suspended mineral cross sections would therefore be expected to display a strong dependence upon geographic location. The suspended inorganic matter indigenous to Lakes Ontario and Ladoga display similar absorption cross section spectra, characterized by minima in the 590-630 nm interval and by maxima at shorter wavelengths. The backscattering cross section spectra determined for the two lakes, however, display distinct

differences in spectral shape. Suspended minerals in Lake Ontario display increased backscattering at short wavelengths as compared to the decreased backscattering displayed by suspended minerals in Lake Ladoga. Both types of suspended minerals, however, display decreasing backscatter in the wavelength interval 550 - 700 nm.

Similarly, Figure 8 compares the absorption cross sections for dissolved organic carbon in Lake Ladoga with the DOC absorption cross sections observed earlier for Lake Ontario. Near-identical spectral slopes were observed in each lake.

The absorption and backscattering cross section spectra for indigenous chlorophyll in Lakes Ladoga and Ontario are compared in Figures 9 and 10, respectively. Morel and Bricaud (1981) have shown that large variations in absorptive properties of chlorophyll may result not only from the many distinct algal species, but also from variations (cell size, cell structure, cell age, cell light history), within the same species. The near identical Lake Ladoga and Lake Ontario chlorophyll absorption cross section spectra of Figure 9 and the very similar backscattering cross section spectra of Figure 10 (which would be even more sensitive to variations in the physical characteristics of the cell than would the absorption cross section spectra) suggests that Lakes Ladoga and Ontario are characterized by optically-comparable populations of chlorophyll-bearing biota.

CONCLUDING REMARKS

The subsurface volume reflectance spectrum observed in a natural water body is a convoluted consequence of the scattering and absorption centres residing within that natural water body. The level

of optical complexity is a direct consequence of the number and nature of the competitive scattering and absorption centres indigenous to the aquatic locale. Consequently, water masses (such as lakes, rivers, estuaries, oceanic coastal regions) containing terrigenous material possess, in general, a considerably higher order optical complexity than will off-shore and mid-oceanic water masses.

An optical water quality model designed to simultaneously extract concentrations of suspended organics, suspended inorganics, and dissolved organics from a single measurement of a subsurface volume reflectance spectrum has been very briefly described. The linkages between the volume reflectance spectrum and the organic and inorganic components of the water mass are provided by the optical cross sections (amount of scattering and absorption per unit concentration of each optically-active aquatic component). Optical cross section spectra for chlorophyll (uncorrected for phaeophytin), suspended minerals, and dissolved organic carbon have been determined for Lake Ontario as well as for Lake Ladoga.

The optical water quality model currently in use in both lakes assumes that at any instant of time a natural water mass may be defined as a homogeneous combination of pure water, unique suspended organic material (represented by the chlorophyll a concentration), unique suspended organic material (represented by the suspended mineral concentration), and dissolved organic material (represented by dissolved organic carbon concentration). Obviously, the definitive model should consider the cross sections of every distinct aquatic component present in natural water masses, as well as any temporally-varying characteristics of these components. Such a model is clearly unattainable. However, an extension to a reasonable number

of additional components would certainly appear to be possible.

Since the water mass is assumed homogeneous, the current model does not include layering effects. Also, no provision is incorporated for chemical impurities. Small concentrations of most chemicals (by comparison with the concentrations of chlorophyll, suspended minerals, and dissolved organic carbon) produce negligible absorption and scattering effects and their detection is beyond current *in situ* optical measurement techniques.

The ability to extract estimates of the concentrations of optically-competitive components of natural waters is of obvious significance to programs which incorporate the remote sensing of environmental parameters. The role of optical cross sections in estimating water quality from space will be further explored in the companion paper.

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FIGURE CAPTIONS

Figure 1: Flow diagram outlining the activities in the development of water quality model based on the specific absorption and scattering cross sections of aquatic components.

Figure 2: Calculated absorption cross sections for chlorophyll a (uncorrected for phaeophytin contamination), total suspended minerals, and dissolved organic carbon. Also shown are the absorption coefficients of pure water.

Figure 3: Calculated scattering cross sections for chlorophyll a (uncorrected for phaeophytin contamination) and total suspended minerals. Also shown are the scattering coefficients of pure water.

Figure 4: Representative examples of directly measured subsurface irradiance reflectance (volume reflectance) spectra obtained at nearshore and midlake stations in Lake Ontario throughout the field season.

Figure 5: Comparison between the calculated "best fit" and directly measured subsurface irradiance reflectance (volume reflectance) spectra for a Niagara River plume station in western Lake Ontario.

Figure 6: Absorption cross sections for suspended minerals calculated for Lake Ladoga. Also shown are the cross sections determined for Lake Ontario a decade earlier.

Figure 7: Backscattering cross sections for suspended minerals calculated for Lake Ladoga. Also shown are the cross sections determined for Lake Ontario a decade earlier.

Figure 8: Absorption cross sections for dissolved organic carbon calculated for Lake Ladoga. Also shown are the cross sections determined for Lake Ontario a decade earlier.

Figure 9: Absorption cross sections for chlorophyll a calculated for Lake Ladoga. Also shown are the cross sections determined for Lake Ontario a decade earlier.

Figure 10: Backscattering cross sections for chlorophyll a calculated for Lake Ladoga. Also shown are the cross sections determined for Lake Ontario a decade earlier.

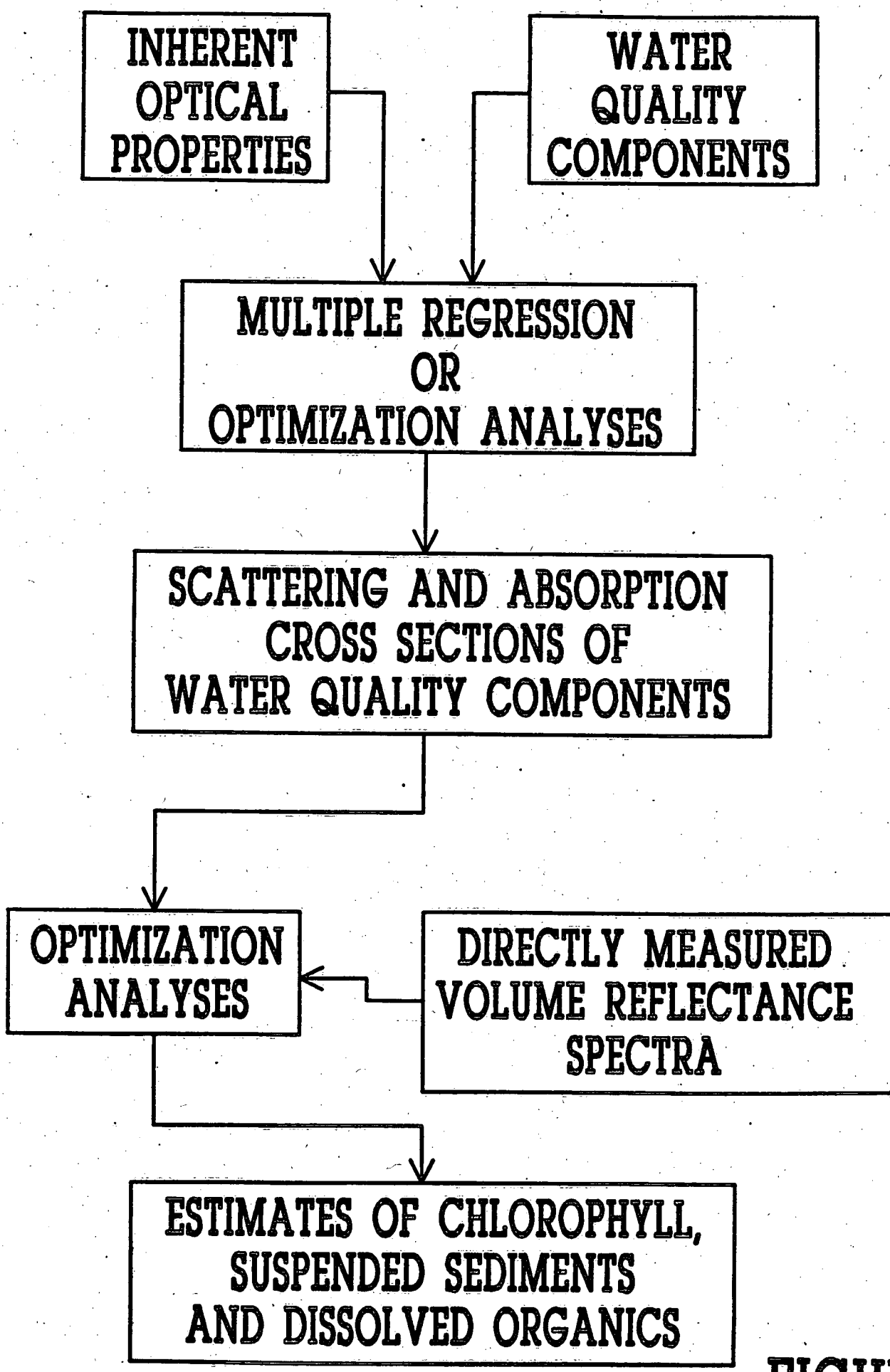
INHERENT OPTICAL PROPERTIES
WATER QUALITY COMPONENTS
MULTIPLE REGRESSION OR OPTIMIZATION ANALYSES
SCATTERING AND ABSORPTION CROSS SECTIONS OF WATER QUALITY COMPONENTS
OPTIMIZATION ANALYSES
DIRECTLY MEASURED VOLUME REFLECTANCE SPECTRA
ESTIMATES OF CHLOROPHYLL, SUSPENDED SEDIMENTS AND DISSOLVED ORGANICS

FIGURE 1

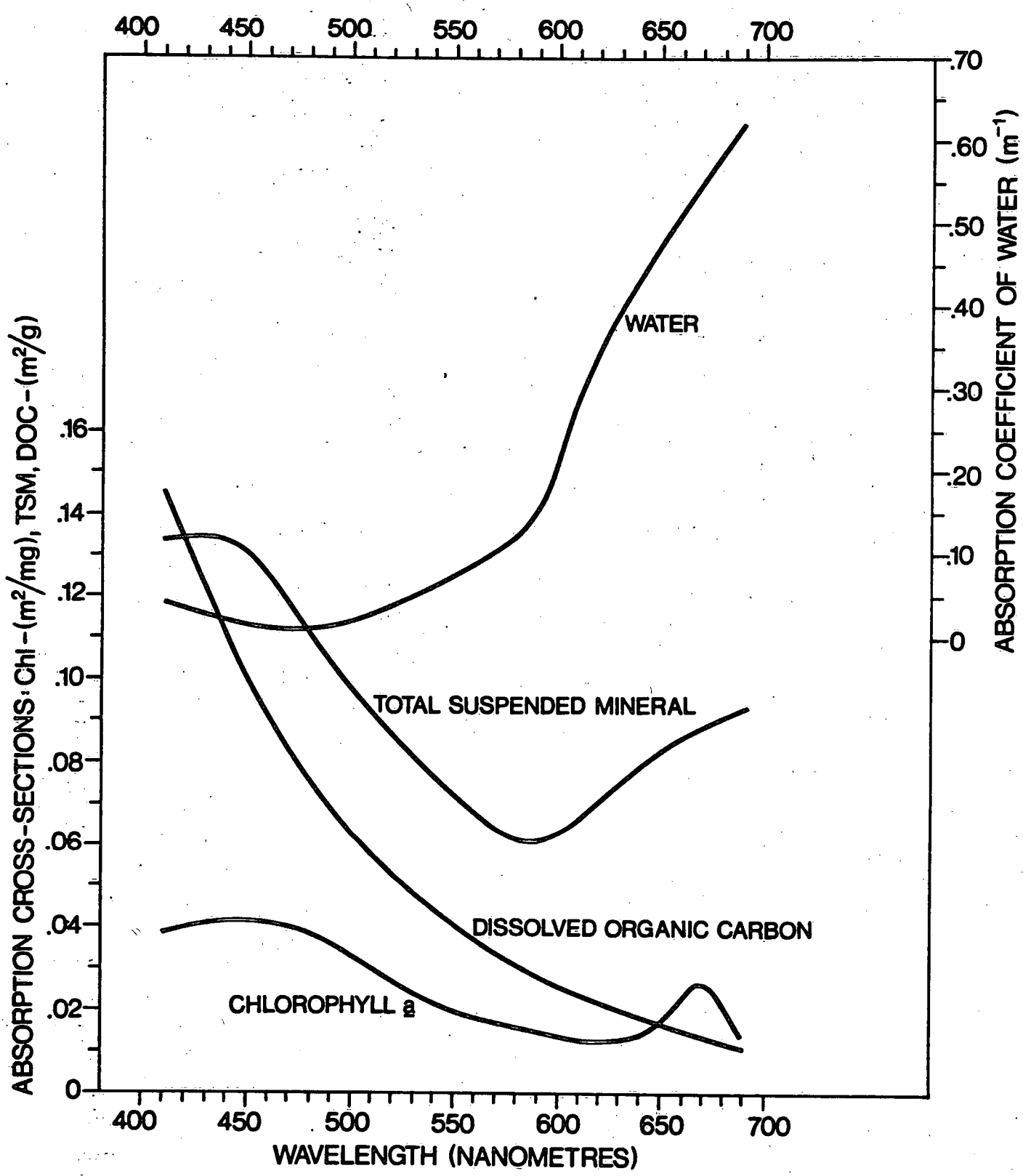
400
450
500
550
600
650
700
.70
.60
.50
.40
.30
.20
.10
0
ABSORPTION COEFFICIENT OF WATER (m^{-1})
WATER
.16
.14
.12
.10
.08
.06
.04
.02
0
ABSORPTION CROSS-SECTIONS: Chl-(m^2/mg), TSM, DOC-(m^2/g)
TOTAL SUSPENDED MINERAL
DISSOLVED ORGANIC CARBON
CHLOROPHYLL a
WAVELENGTH (NANOMETRES)

FIGURE 2

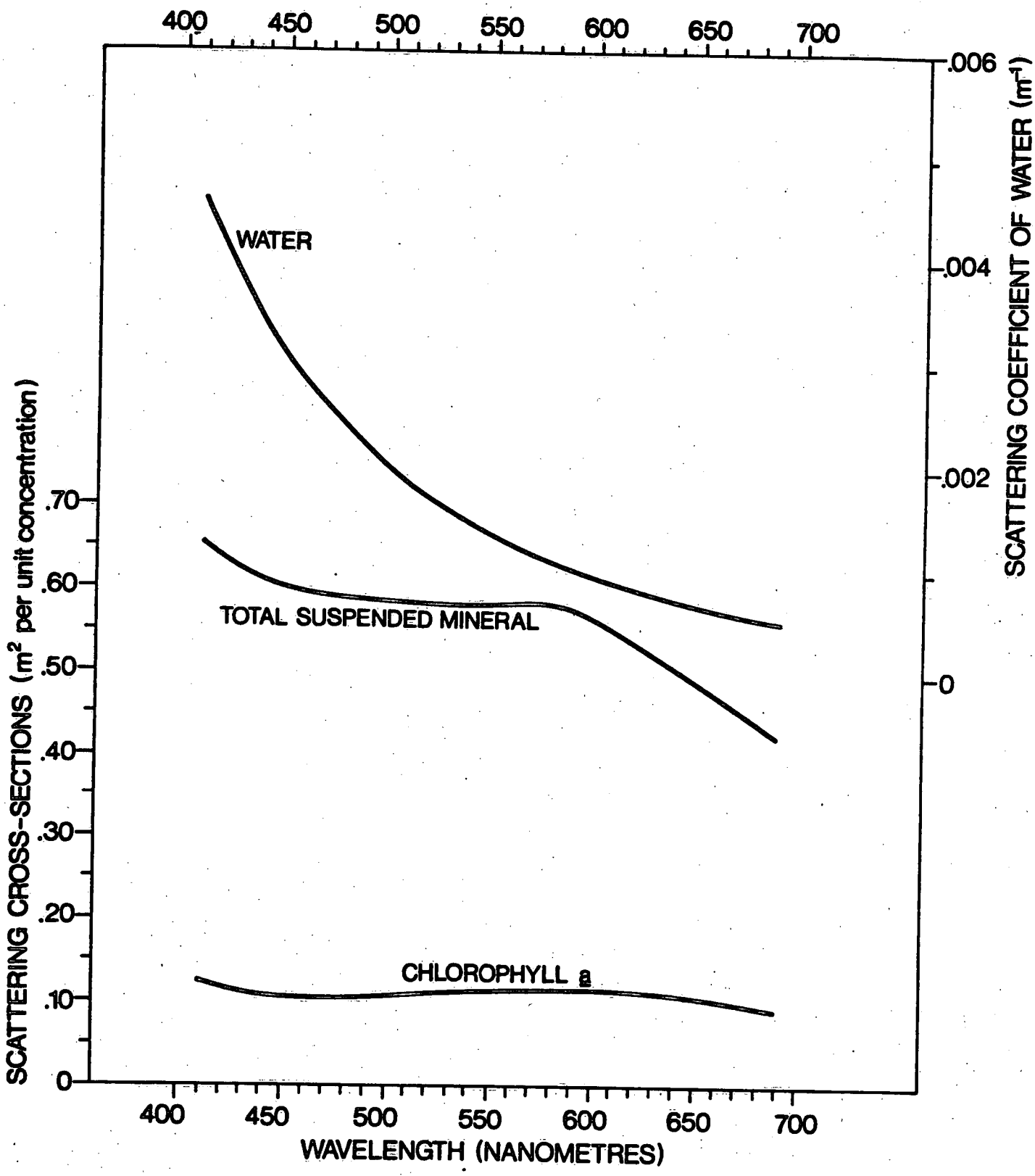
400
450
500
550
600
650
700
.006
.004
.002
0
SCATTERING COEFFICIENT OF WATER (m⁻¹)
WATER
TOTAL SUSPENDED MINERAL
CHLOROPHYLL a
.70
.60
.50
.40
.30
.20
.10
0
SCATTERING CROSS-SECTIONS (m² per unit concentration)
WAVELENGTH (NANOMETRES)

FIGURE 3

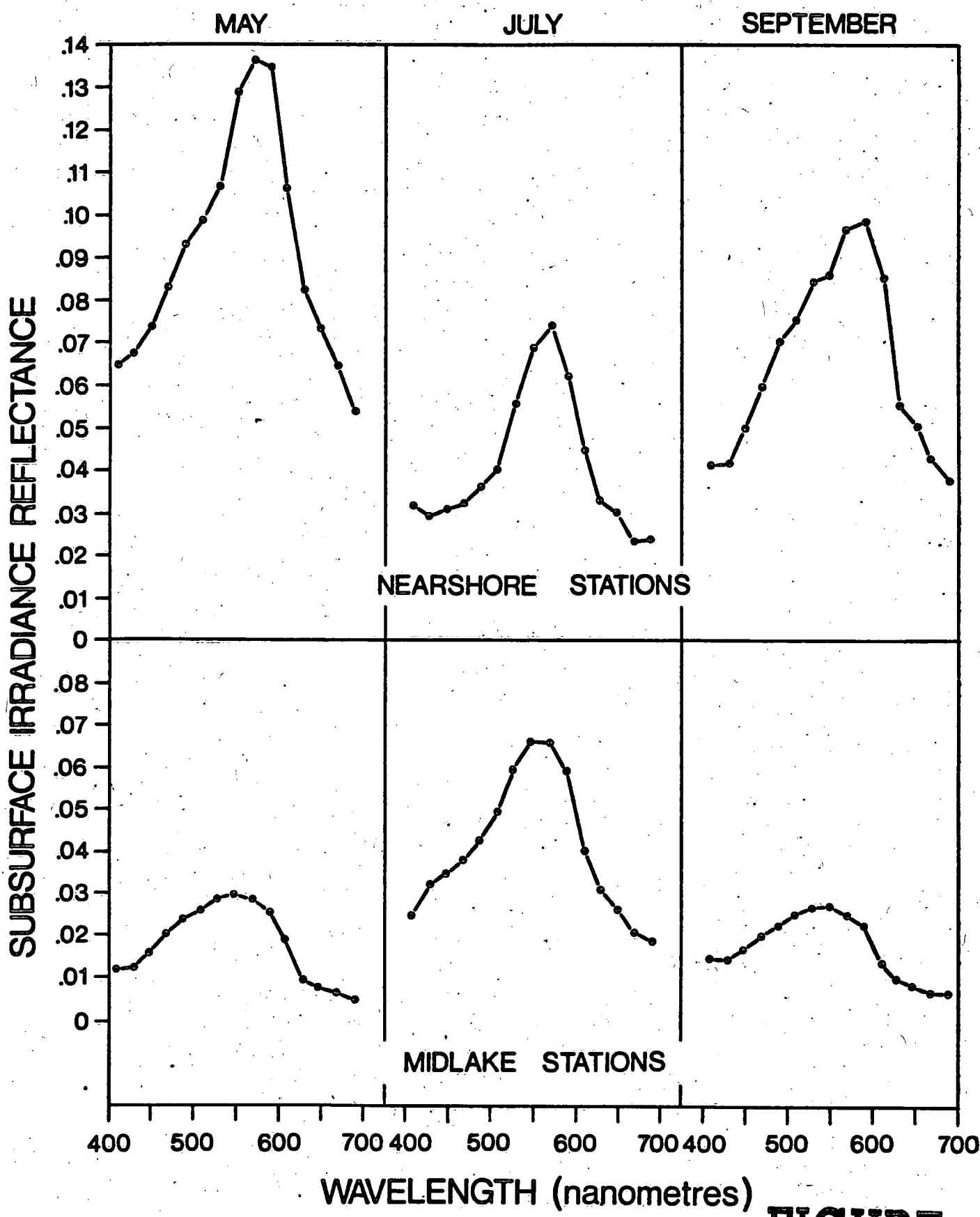
MAY
JULY
SEPTEMBER
SUBSURFACE IRRADIANCE REFLECTANCE
.14
.13
.12
.11
.10
.09
.08
.07
.06
.05
.04
.03
.02
.01
0
NEARSHORE STATIONS
.08
.07
.06
.05
.04
.03
.02
.01
0
MIDLAKE STATIONS
400
500
600
700
WAVELENGTH (nanometres)

FIGURE 4

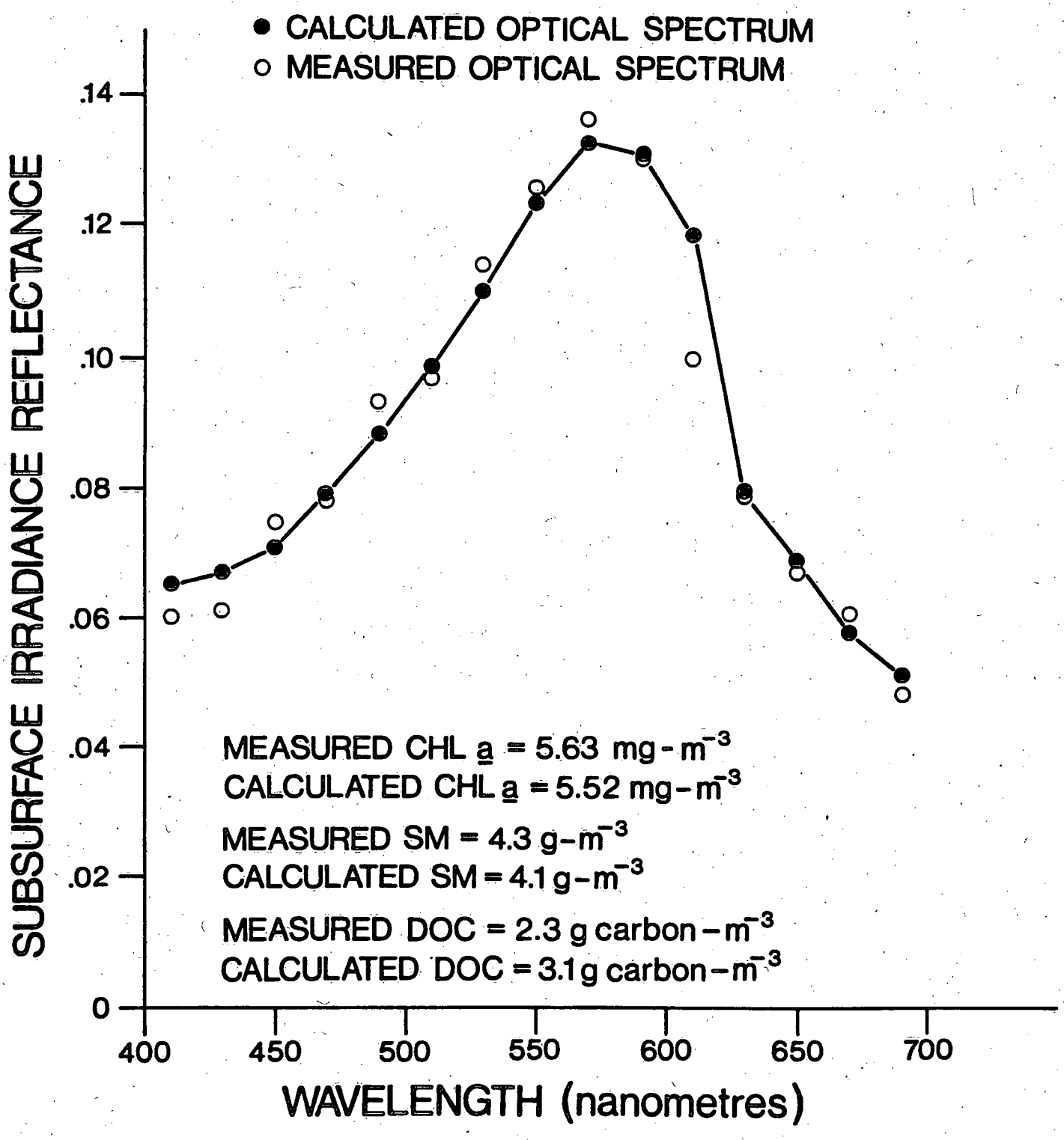
● CALCULATED OPTICAL SPECTRUM
○ MEASURED OPTICAL SPECTRUM
SUBSURFACE IRRADIANCE REFLECTANCE
.14
.12
.10
.08
.06
.04
.02
0
400
450
500
550
600
650
700
WAVELENGTH (nanometres)
MEASURED CHL a = 5.63 mg-m^{-3}
CALCULATED CHL a = 5.52 mg-m^{-3}
MEASURED SM = 4.3 g-m^{-3}
CALCULATED SM = 4.1 g-m^{-3}
MEASURED DOC = 2.3 g carbon-m^{-3}
CALCULATED DOC = 3.1 g carbon-m^{-3}

FIGURE 5

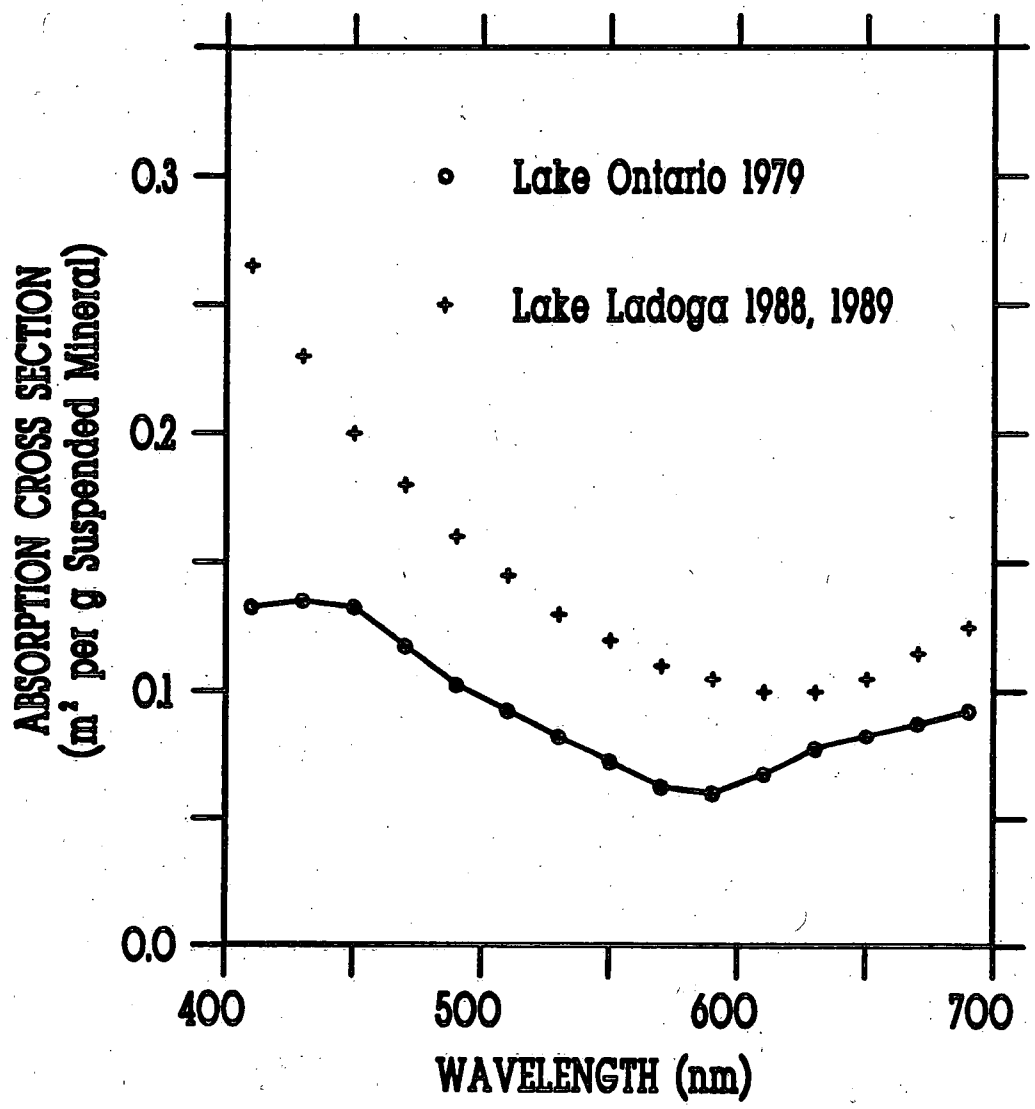
Lake Ontario 1979
Lake Ladoga 1988, 1989
ABSORPTION CROSS SECTION
(m^2 per g Suspended Mineral)
0.3
0.2
0.1
0.0
400
500
600
700
WAVELENGTH (nm)

FIGURE 6

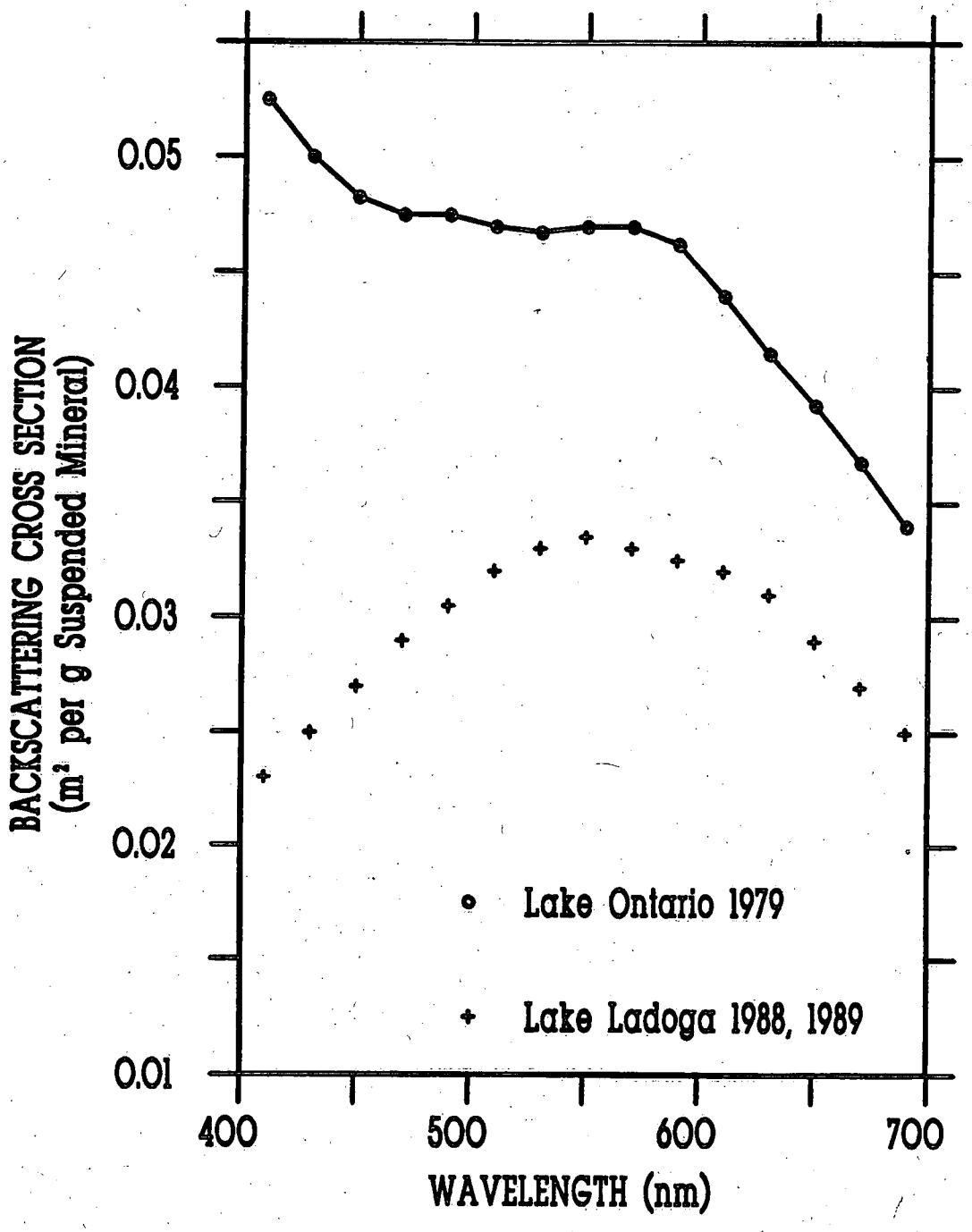
BACKSCATTERING CROSS SECTION
(m² per g Suspended Mineral)
0.05
0.04
0.03
0.02
0.01
400
500
600
700
WAVELENGTH (nm)
Lake Ontario 1979
Lake Ladoga 1988, 1989

FIGURE 7

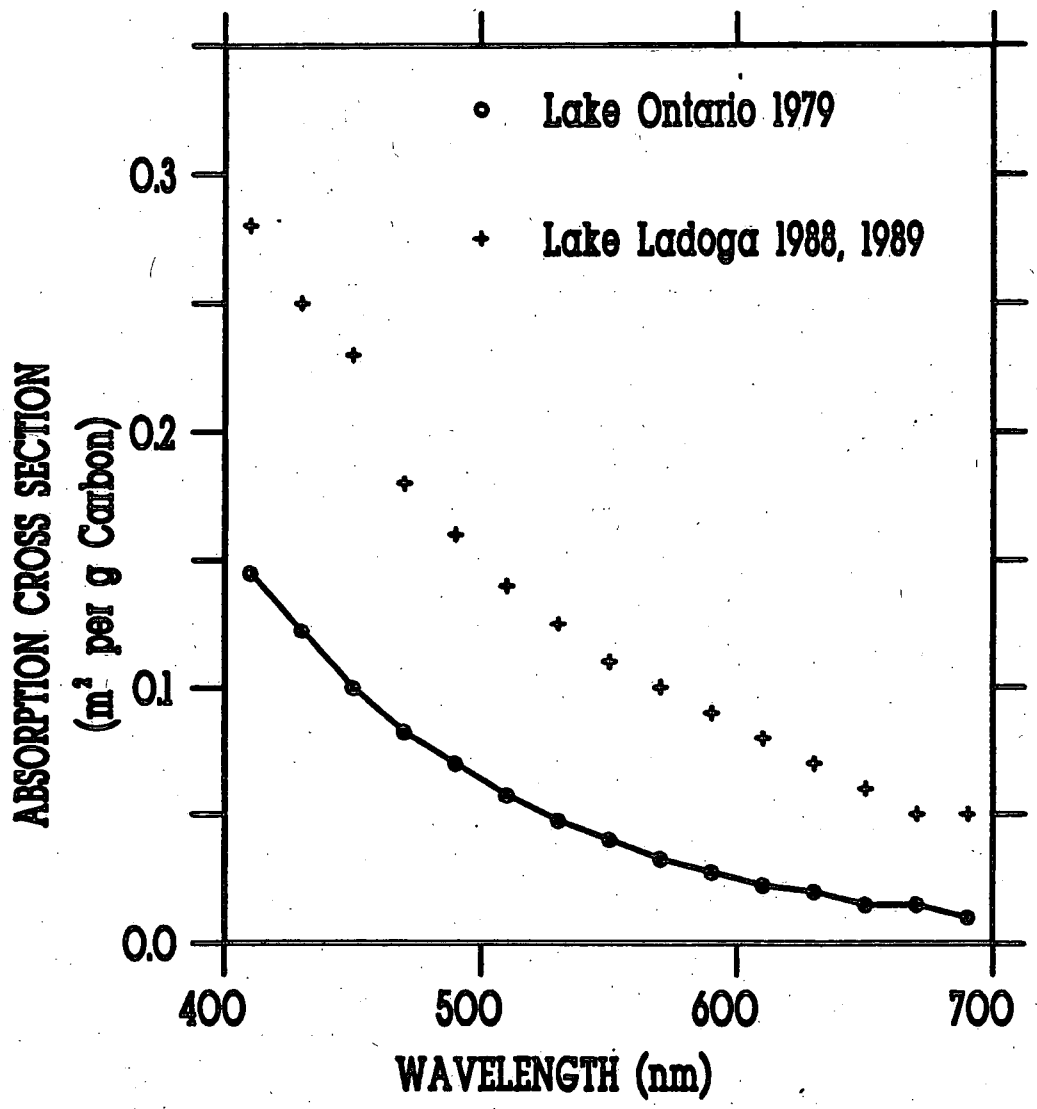
Lake Ontario 1979
Lake Ladoga 1988, 1989
0.3
0.2
0.1
0.0
ABSORPTION CROSS SECTION
(m^2 per g Carbon)
400
500
600
700
WAVELENGTH (nm)

FIGURE 8

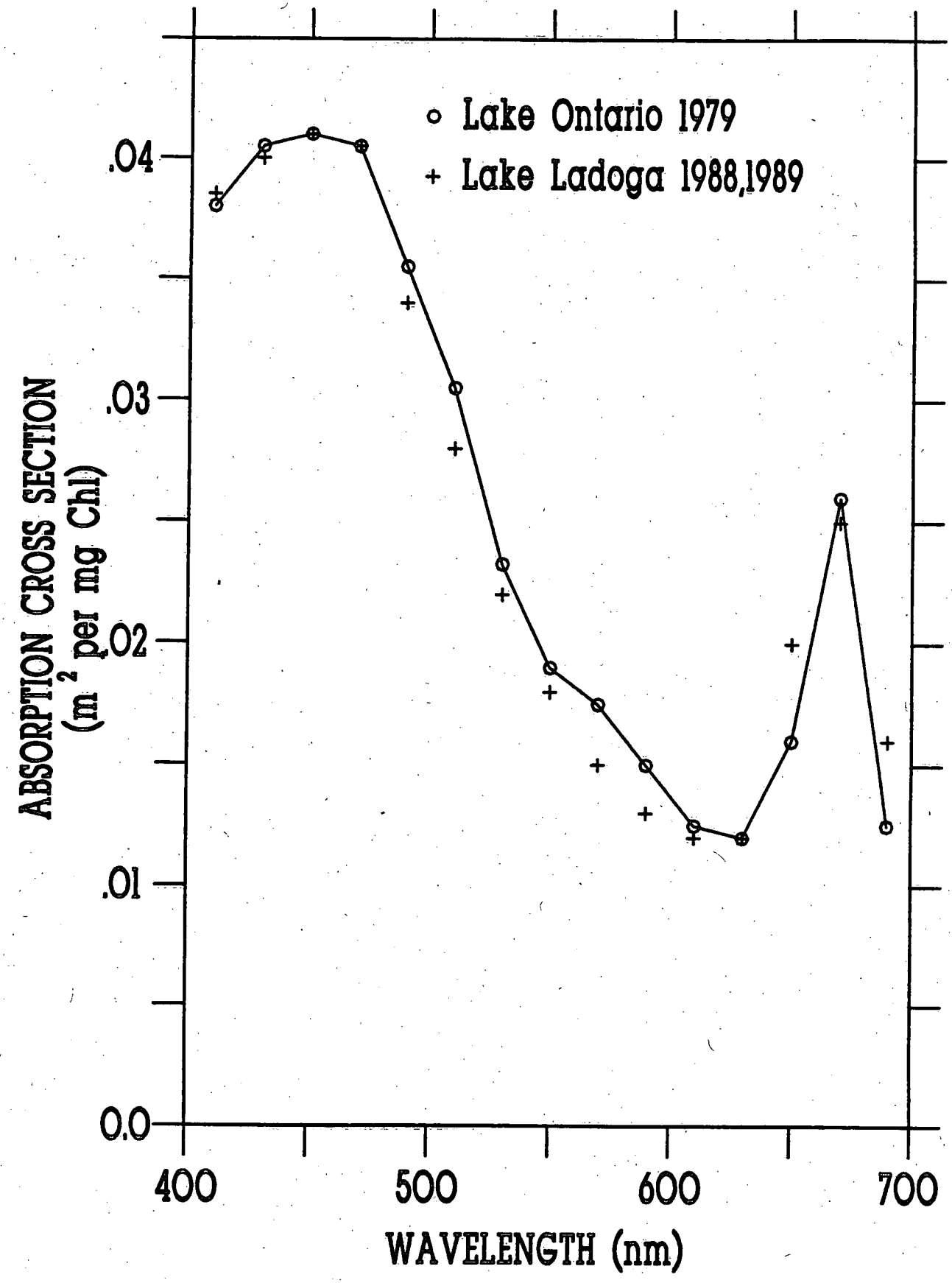
Lake Ontario 1979
Lake Ladoga 1988,1989
ABSORPTION CROSS SECTION
(m 2 per mg Chl)
.04
.03
.02
.01
0.0
400
500
600
700
WAVELENGTH (nm)

FIGURE 9

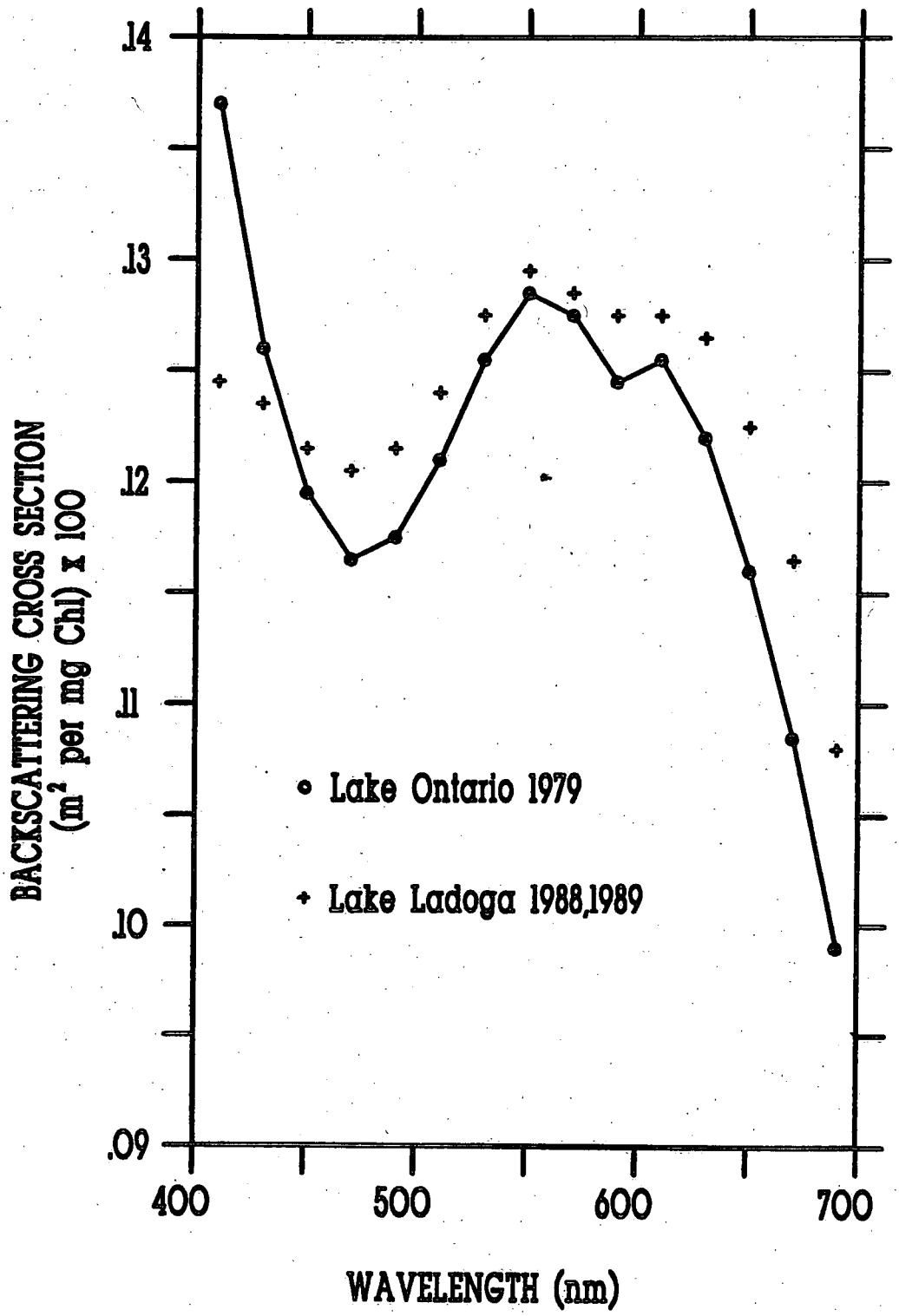
.14
.13
.12
.11
.10
.09
BACKSCATTERING CROSS SECTION
(m^2 per mg Chl) x 100
Lake Ontario 1979
Lake Ladoga 1988,1989
400
500
600
700
WAVELENGTH (nm)

FIGURE 10

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