

Optical Constants of Water in the 200-nm to 200- μ m Wavelength Region

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Extinction coefficients $k(\lambda)$ for water at 25°C were determined through a broad spectral region by manually smoothing a point by point graph of $k(\lambda)$ vs wavelength λ that was plotted for data obtained from a review of the scientific literature on the optical constants of water. Absorption bands representing $k(\lambda)$ were postulated where data were not available in the vacuum uv and soft x-ray regions. A subtractive Kramers-Kronig analysis of the combined postulated and smoothed portions of the $k(\lambda)$ spectrum provided the index of refraction $n(\lambda)$ for the spectral region $200 \text{ nm} \leq \lambda \leq 200 \mu\text{m}$.

I. Introduction

The index of refraction $n(\lambda)$ and the extinction coefficient $k(\lambda)$ of water are, respectively, the real and imaginary parts of its spectral complex refractive index $\tilde{n}(\lambda) = n(\lambda) - ik(\lambda)$, where λ is the wavelength of an electromagnetic wave in vacuum. These physical parameters together with the complex Fresnel equations and the generalized Fresnel equations provide the basis for computing the optical properties of water. In recent years knowledge of the optical properties of water has been of greater interest because of its application in (1) computing radiation transport through atmospheres containing water droplets and other aerosols or through oceans containing hydrosols, (2) development of optical remote sensing instruments for measuring the chemical and thermal quality or turbidity of environmental waters and for measuring the water content of soils, (3) computing the optical properties of plant leaves, and (4) investigations of the optical properties and optical constants of aqueous solutions.

In 1968 Irvine and Pollack¹ published results from a critical review of the existing literature on the optical properties of water for the 0.2–200- μ m wavelength region. They tabulated measured values of both $k(\lambda)$ and the Lambert absorption coefficient $\alpha(\lambda) = 4\pi k(\lambda)/\lambda$ from about thirty different papers appearing in the scientific literature. Next, using the only four reports on measurements of the reflectance of water that were available at that time, they tabulated values for the reflectance $R(\lambda)$ measured at near normal incidence for a free water surface. The tabulated values for $k(\lambda)$ and the generalized

Fresnel reflectance equation for $R(\lambda)$, i.e., the Cauchy equation, then provided values for $n(\lambda)$.

Zolotarev *et al.*² in 1969 reported values for the optical constants of water throughout the spectral region 1–10⁶ μ m. They determined both $k(\lambda)$ and $n(\lambda)$ from their measurements of $\alpha(\lambda)$ and $R(\lambda)$ for water at 25°C in the 2–50- μ m region and measurements of internal reflectance spectra in the 2–10- μ m region. Their measurements and reliable data from thirteen other papers in the scientific literature provided values of $k(\lambda)$ throughout the spectral region 1–10⁶ μ m. Values of $n(\lambda)$ were then obtained from a Kramers-Kronig (K-K) analysis of the $k(\lambda)$ spectrum:

$$n(\lambda_0) = 1 + \frac{2\lambda_0^2}{\pi} \int_0^\infty \frac{k(\lambda)d\lambda}{\lambda(\lambda_0^2 - \lambda^2)}. \quad (1)$$

For making the integration indicated by Eq. (1) a model absorption band with central position at 100 nm was constructed for $k(\lambda)$ in the uv region. The band was reported to have no significant affect on calculated values of $n(\lambda)$ for $\lambda \geq 1 \mu\text{m}$. Zolotarev *et al.* noted discrepancies in the 20–50- μ m region between their values for $n(\lambda)$ and those reported by Irvine and Pollack. They noted that in the 6.5–9- μ m region the values of $k(\lambda)$ measured by Pointier and Dechambenoy³ were 30% smaller than their measured values for that quantity, and also that values for both $n(\lambda)$ and $k(\lambda)$ at the ir band centers were in disagreement with those measured by Pointier and Dechambenoy.

Since Zolotarev *et al.* completed their investigation of the optical constants of water in 1968 at least nine other papers^{4–13} appearing in the literature have reported measurements of the optical properties of water in the vacuum uv, visible, ir, or microwave spectral regions. Of particular interest are the care-

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ful measurements reported by Robertson and Williams⁶ for $\alpha(\lambda)$ in the 2.5–38.4- μm region, and the measurements of reflectance and subsequent computations of $n(\lambda)$ and $k(\lambda)$ reported by Painter *et al.*^{9,10} and Kerr *et al.*⁸ which, when combined, extend through the 80–300-nm region of the vacuum uv.

We felt a need at this time for an updated review of the literature on the optical constants of water (1) because a current knowledge of the optical constants of water is essential to our investigations of aqueous solutions,^{14–15} (2) because of the discrepancies between values reported for both $n(\lambda)$ and $k(\lambda)$, and (3) because of the additional measurements of these quantities that have been reported since 1968 for the ir and uv spectral regions. We therefore compiled values of $k(\lambda)$ from the scientific literature and then point by point plotted graphs of these measured values for $k(\lambda)$ vs λ through the microwave, far ir, ir, visible, x-ray, and part of the uv regions of the electromagnetic spectrum. A smooth continuous curve for $k(\lambda)$ then was drawn manually through the plotted points. Values for $k(\lambda)$ were postulated in the vacuum uv and soft x-ray regions where data were not available from the literature. A subtractive Kramers-Kronig (K-K) analysis of the $k(\lambda)$ spectrum then provided values of $n(\lambda)$ for the spectral region $200\text{ nm} \leq \lambda \leq 200\text{ }\mu\text{m}$.

II. Acquisition of Data

A search was made for literature reporting measurements of the electromagnetic absorption characteristics of liquid water in any spectral region. Fifty-eight articles and books^{1–13,16–59} were selected from the literature of the past 81 years. The selected references were examined individually for specific values or for graphical or tabulated values of the extinction coefficient $k(\lambda)$; Lambert absorption coefficient $\alpha(\lambda) = 4\pi k(\lambda)/\lambda$; molecular absorption coefficient $\xi(\lambda)_m = \alpha(\lambda)/(2.3026C)$, where C is the concentration of the substance in units of moles/liter; absorption index $K(\lambda) = k(\lambda)/n(\lambda)$; real $\xi_r(\lambda) = 2n(\lambda)k(\lambda)$ and imaginary $\xi_i(\lambda) = n(\lambda)^2 - k(\lambda)^2$ parts of the complex dielectric constant; or mass absorption coefficient $(\mu/\rho)_k = 4\pi k(\lambda)/\lambda\rho$, where $\rho = 1\text{ g/cm}^3$. A listing of all accumulated values for $k(\lambda)$ ordered with respect to increasing λ was provided by an IBM 360/50 computer. In many cases significant discrepancies were noted between values of $k(\lambda)$ at the same λ but obtained from different references. All points in the listing then were plotted manually on graphs of $k(\lambda)$ vs λ . The best visual fit to the plotted data for $k(\lambda)$ was obtained by manually drawing a smooth curve through the points while weighting the curve in favor of data for water at 25°C and in favor of data reported by authors who in our judgment used careful experimental procedures. Two postulated absorption bands of Gaussian shape were constructed for $k(\lambda)$ in the soft x-ray and vacuum uv regions where data were not available from the literature. The final values for $k(\lambda)$ are shown graphically by the solid-line curves in Figs. 1–5 and

are tabulated in Table I at selected positions between 200 nm and 200 μm .

III. Discussion of Graphs for $k(\lambda)$ vs λ

A. Figure 1, Graph 0–0.5 Å

The smooth curve shown in this graph was based on values for absorption coefficients of water for x rays and γ rays as reported by Allen.²⁷

B. Figure 1, Graph 0–55 Å

The smooth solid-line curve shown in this graph was based on values for the absorption coefficients of x rays and γ rays as reported by Allen²⁷ for the 0.25–0.7-Å region and values for the mass absorption coefficients taken from Ref. 52 for the 0.71–2.5-Å region and from Engstrom⁵¹ for the 5–22-Å region. The smooth dashed-line curve was the short wavelength side of an absorption band postulated for $k(\lambda)$ in the soft x-ray region.

C. Figure 1, Graph 0–2000 Å

1. Spectral Region 22–849 Å

Data for this region were not available from the literature. The dashed-line curve for $k(\lambda)$ in this region was postulated in the following subjective manner: The curve was made Gaussian shaped between 850 Å and about 300 Å. The band with peak value at about 80 Å was added in order to join continuously the solid-line curve ending at 22 Å with the Gaussian shaped curve at about 300 Å.

2. Spectral Region 849–1250 Å

The only data available for this region were those of Kerr *et al.*⁸ (KHW). Their values for $k(\lambda)$ were calculated by K-K analysis of reflectance data for water at 1°C. For $\lambda \geq 1250\text{ Å}$ their values of $k(\lambda)$ are greater than those reported by other investigators. Therefore, we chose for this region the similar shaped but smaller-in-magnitude dashed-line curve that was thought to represent $k(\lambda)$ for water at 25°C.

3. Spectral Region 1250–2000 Å

The heavy solid-line curve was based on data from Painter *et al.*^{9,10} and data from Refs. 42, 44, 46, 47, and 49. Because the curve is rapidly rising in the 1700–1850-Å region, individual values of $k(\lambda)$ read from this curve are subject to a significant amount of error.

D. Figure 2, Graph 180–1000 nm

The smooth solid-line curve was based mostly on values of $k(\lambda)$ from Refs. 11, 16–19, 31, 34, and 40. Notable exceptions to the curve selected for $k(\lambda)$ are data of Lenoble and Saint-Guilly³¹ (LSG) and of Tyler *et al.*¹¹ (TSW). The paper by TSW was a recent one predicting the optical properties of clear natural water. Data reported by LSG, when compared to our curve, are lower for $\lambda < 370\text{ nm}$ and are greater for $\lambda > 370\text{ nm}$. At 400 nm, values of $k(\lambda)$ from LSG were significantly greater than values of $k(\lambda)$ from Clarke and James⁴⁰ (CJ) and from several

Table 1. Optical Constants of Water

$\lambda(\mu\text{m})$	$k(\lambda)$	$n(\lambda)$	$\lambda(\mu\text{m})$	$k(\lambda)$	$n(\lambda)$	$\lambda(\mu\text{m})$	$k(\lambda)$	$n(\lambda)$
0.200	1.1×10^{-7}	1.396	3.40	0.0195	1.420	9.8	0.0479	1.229
0.225	4.9×10^{-8}	1.373	3.45	0.0132	1.410	10.0	0.0508	1.218
0.250	3.35×10^{-8}	1.362	3.50	0.0094	1.400	10.5	0.0662	1.185
0.275	2.35×10^{-8}	1.354	3.6	0.00515	1.385	11.0	0.0968	1.153
0.300	1.6×10^{-8}	1.349	3.7	0.00360	1.374	11.5	0.142	1.126
0.325	1.08×10^{-8}	1.346	3.8	0.00340	1.364	12.0	0.199	1.111
0.350	6.5×10^{-9}	1.343	3.9	0.00380	1.357	12.5	0.259	1.123
0.375	3.5×10^{-9}	1.341	4.0	0.00460	1.351	13.0	0.305	1.146
0.400	1.86×10^{-9}	1.339	4.1	0.00562	1.346	13.5	0.343	1.177
0.425	1.3×10^{-9}	1.338	4.2	0.00688	1.342	14.0	0.370	1.210
0.450	1.02×10^{-9}	1.337	4.3	0.00845	1.338	14.5	0.388	1.241
0.475	9.35×10^{-10}	1.336	4.4	0.0103	1.334	15.0	0.402	1.270
0.500	1.00×10^{-9}	1.335	4.5	0.0134	1.332	15.5	0.414	1.297
0.525	1.32×10^{-9}	1.334	4.6	0.0147	1.330	16.0	0.422	1.325
0.550	1.96×10^{-9}	1.333	4.7	0.0157	1.330	16.5	0.428	1.351
0.575	3.60×10^{-9}	1.333	4.8	0.0150	1.330	17.0	0.429	1.376
0.600	1.09×10^{-8}	1.332	4.9	0.0137	1.328	17.5	0.429	1.401
0.625	1.39×10^{-8}	1.332	5.0	0.0124	1.325	18.0	0.426	1.423
0.650	1.64×10^{-8}	1.331	5.1	0.0111	1.322	18.5	0.421	1.443
0.675	2.23×10^{-8}	1.331	5.2	0.0101	1.317	19.0	0.414	1.461
0.700	3.35×10^{-8}	1.331	5.3	0.0098	1.312	19.5	0.404	1.476
0.725	9.15×10^{-8}	1.330	5.4	0.0103	1.305	20.0	0.393	1.480
0.750	1.56×10^{-7}	1.330	5.5	0.0116	1.298	21.0	0.382	1.487
0.775	1.48×10^{-7}	1.330	5.6	0.0142	1.289	22	0.373	1.500
0.800	1.25×10^{-7}	1.329	5.7	0.0203	1.277	23	0.367	1.511
0.825	1.82×10^{-7}	1.329	5.8	0.0330	1.262	24	0.361	1.521
0.850	2.93×10^{-7}	1.329	5.9	0.0622	1.248	25	0.356	1.531
0.875	3.91×10^{-7}	1.328	6.0	0.107	1.265	26	0.350	1.539
0.900	4.86×10^{-7}	1.328	6.1	0.131	1.319	27	0.344	1.545
0.925	1.06×10^{-6}	1.328	6.2	0.0880	1.363	28	0.338	1.549
0.950	2.93×10^{-6}	1.327	6.3	0.0570	1.357	29	0.333	1.551
0.975	3.48×10^{-6}	1.327	6.4	0.0449	1.347	30	0.328	1.551
1.0	2.89×10^{-6}	1.327	6.5	0.0392	1.339	32	0.324	1.546
1.2	9.89×10^{-6}	1.324	6.6	0.0356	1.334	34	0.329	1.536
1.4	1.38×10^{-4}	1.321	6.7	0.0337	1.329	36	0.343	1.527
1.6	8.55×10^{-5}	1.317	6.8	0.0327	1.324	38	0.361	1.522
1.8	1.15×10^{-4}	1.312	6.9	0.0322	1.321	40	0.385	1.519
2.0	1.1×10^{-3}	1.306	7.0	0.0320	1.317	42	0.409	1.522
2.2	2.89×10^{-4}	1.296	7.1	0.0320	1.314	44	0.436	1.530
2.4	9.56×10^{-4}	1.279	7.2	0.0321	1.312	46	0.462	1.541
2.6	3.17×10^{-3}	1.242	7.3	0.0322	1.309	48	0.488	1.555
2.65	6.7×10^{-3}	1.219	7.4	0.0324	1.307	50	0.514	1.587
2.70	0.019	1.188	7.5	0.0326	1.304	60	0.587	1.703
2.75	0.059	1.157	7.6	0.0328	1.302	70	0.576	1.821
2.80	0.115	1.142	7.7	0.0331	1.299	80	0.547	1.886
2.85	0.185	1.149	7.8	0.0335	1.297	90	0.536	1.924
2.90	0.268	1.201	7.9	0.0339	1.294	100	0.532	1.957
2.95	0.298	1.292	8.0	0.0343	1.291	110	0.531	1.966
3.00	0.272	1.371	8.2	0.0351	1.286	120	0.526	2.004
3.05	0.240	1.426	8.4	0.0361	1.281	130	0.514	2.036
3.10	0.192	1.467	8.6	0.0372	1.275	140	0.500	2.056
3.15	0.135	1.483	8.8	0.0385	1.269	150	0.495	2.069
3.20	0.0924	1.478	9.0	0.0399	1.262	160	0.496	2.081
3.25	0.0610	1.467	9.2	0.0415	1.255	170	0.497	2.094
3.30	0.0368	1.450	9.4	0.0433	1.247	180	0.499	2.107
3.35	0.0261	1.432	9.6	0.0454	1.239	190	0.501	2.119
						200	0.504	2.130

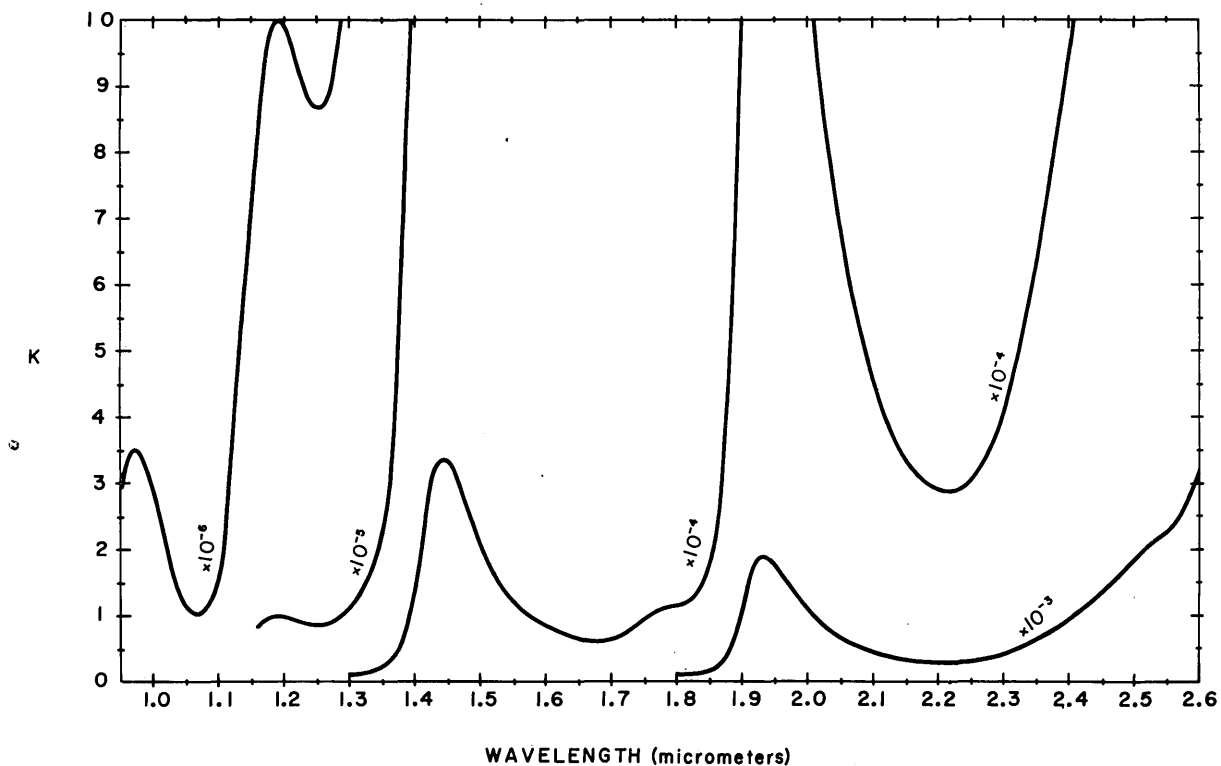


Fig. 3. Extinction coefficients of water for the 0.95–2.6- μ m spectral region. Curves are described in the text.

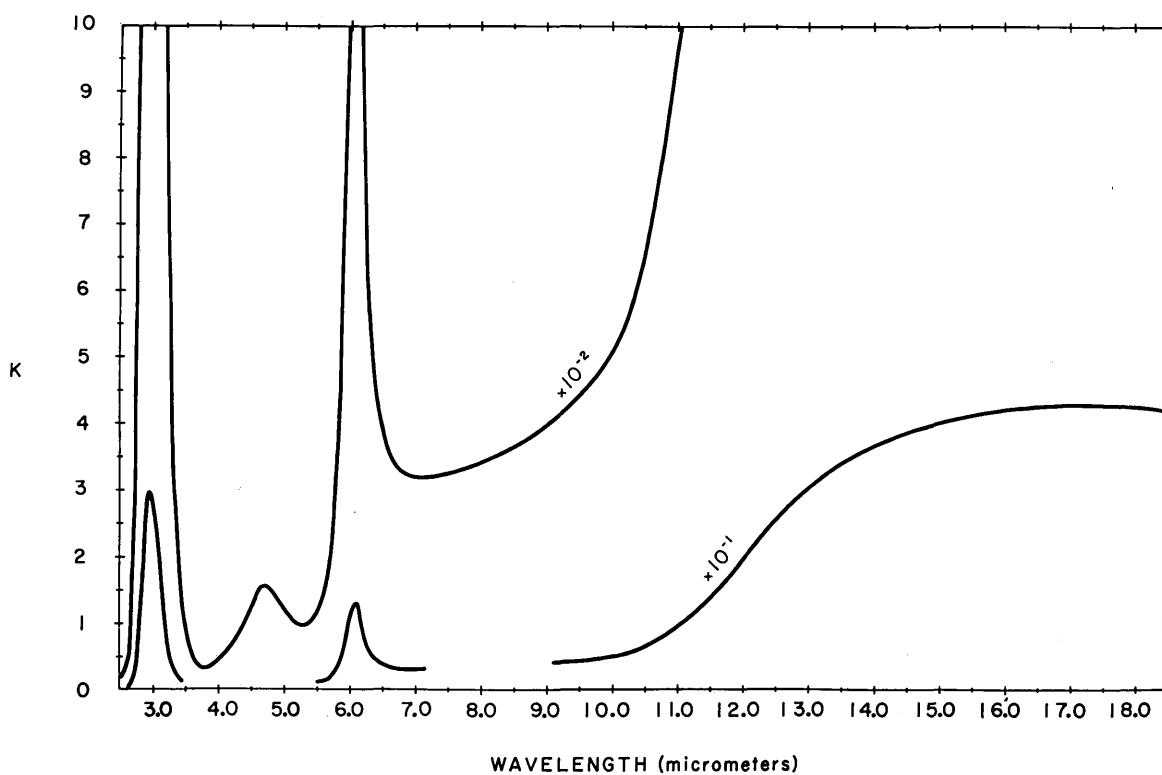


Fig. 4. Extinction coefficients of water for the 2.5–18.5- μ m spectral region. Curves are described in the text.

of the other references. Data from CJ suggested a more highly structured curve for $k(\lambda)$ than the one we constructed in the 380–580-nm region, but the scatter of data from other references allowed only the selected curve. Sullivan¹⁸ provided a consistent set of data for $k(\lambda)$ throughout the region 580–790 nm. The structure of our curve for $k(\lambda)$, however, departed slightly from that suggested by Sullivan's data in the region of the maximum for $k(\lambda)$ at about 760 nm. In the 800–1000-nm region the curve for $k(\lambda)$ was based primarily on data from Curcio and Petty³⁴ and Kondratyev.¹⁹ Values for $k(\lambda)$ from data reported by Bayly *et al.*²⁶ seemed to be consistently too large.

E. Figure 3, Graph 0.95–2.6 μm

The smooth solid-line curve for $k(\lambda)$ was based on data from Refs. 1–7, 16, 17, 19, 20, 23, 25, 28, 34, 39, 53, and 54. In the 0.95–2.0- μm region the primary references were Kondratyev,¹⁹ Curcio and Petty,³⁴ and Zolotarev *et al.*² In the 2.0–2.6- μm region Centeno's data were in poor agreement with data from several of the other references. The small shoulder band at 2.5 μm originally reported by Collins³⁹ and recently commented on by Robertson and Williams⁶ was included in our curve for $k(\lambda)$.

F. Figure 4, Graph 2.5–18.5 μm

The smooth solid-line curve for $k(\lambda)$ was based on data from Refs. 1–7, 17, 19, 23, 25, 26, 28, 29, 38, and 54. The better data seemed to be those of Robertson and Williams⁶ and Zolotarev *et al.*² The maximum value of $k(\lambda)$, $k(17.2 \mu\text{m}) = 0.430$, for the liberation band was estimated in both position and magnitude from data of Hale *et al.*⁷ Values of $k(\lambda)$ from Irvine and Pollack¹ agree fairly well with the curve selected through this spectral region.

G. Figure 5, Graph 10–100 μm

Data through this spectral region were selected from Refs. 1–7, 17, 19, 22, 24, 28, 29, 50, and 54. Many discrepancies existed between values for $k(\lambda)$ reported by different investigators. Data from Rusk *et al.*⁵ (RWQ) seemed to assign values for $k(\lambda)$ that were too large; this was attributed to an inefficient polarizer for $\lambda > 20 \mu\text{m}$. Data from Robertson and Williams⁶ (ROW) seemed to assign values for $k(\lambda)$ that were too small; as noted in the original paper this was perhaps due in part to scattered radiant flux that remained undetected. Temperature influences the shape and position of the libration band as indicated by Hale *et al.*⁷ and by Pointier and Dechambenois³ (PD, 1966). Temperature of the water was not indicated by ROW. Our smooth curve for $k(\lambda)$ was based on a median estimate between ROW and PD; the estimate coincides very well with data from Zolotarev *et al.*² In the 58–84- μm region the curve for $k(\lambda)$ follows closely data from Draegert *et al.*,²² Zolotarev *et al.*,² and Irvine and Pollack.¹ Above 84 μm the curve was primarily based on data from Zolotarev *et al.*

H. Figure 5, Graph 50–100 μm

Data from Chamberlain *et al.*²¹ and their references and from Zolotarev *et al.*² were used for $k(\lambda)$ in this spectral region.

I. Figure 5, Graph 0–10 cm

Data from Rabinovich and Melentyev¹³ (RBM) and from Zolotarev *et al.*² and from Refs. 12, 19, 30, 32, 35, and 41 were used for $k(\lambda)$ in this spectral region.

J. Figure 5, Graph 0–1.0 m (curve begins at 10 cm)

The solid-line curve was a smooth fit to scattered data points selected from Refs. 2 and 37. There were probably some regions of absorption that were not shown in the final curve.

IV. Index of Refraction

Values of the index of refraction $n(\lambda)$ for the spectral region 200 nm to 200 μm were computed by applying a subtractive Kramers-Kronig analysis^{58,59} (SKK) to the continuous spectrum for $k(\lambda)$ shown in Figs. 1–5. Accordingly, the index of refraction $n(\lambda_0)$ at wavelength λ_0 is

$$n(\lambda_0) = n(\lambda_1) + \text{Prin.} \left[\frac{2(\lambda_1^2 - \lambda_0^2)}{\pi} \int_0^\infty \frac{\lambda k(\lambda) d\lambda}{(\lambda_0^2 - \lambda^2)(\lambda_1^2 - \lambda^2)} \right], \quad (2)$$

where $n(\lambda_1)$ is a known value for the index of refraction at wavelength λ_1 , and Prin. denotes the Cauchy principal value of the integral. The integral was evaluated throughout the 10^{-4} -nm to 1-m region by use of a combination of Simpson's rule and trapezoidal numerical approximations that were programmed in Fortran IV for an IBM 360/50 computer. Contributions to the integral for $\lambda \leq 10^{-4}$ nm were assumed to be negligible, and those for $\lambda \geq 1$ m were obtained analytically by assuming $k(\lambda) = k(1\text{m})$ throughout the region $\lambda \geq 1$ m. It also was advantageous to choose λ_1 so that it did not coincide with λ at any point during the sequence of numerical approximations. We chose⁵² $n(\lambda_1) = n(589.3 \text{ nm}) = 1.3325$, whereas the data contained values of $k(\lambda)$ at 585 nm and 590 nm. Values for $n(\lambda)$ resulting from these integration procedures are given in Table I and are shown graphically by the solid-line curves in Fig. 6.

The influence of the shape and height of the postulated uv and soft x-ray bands for $k(\lambda)$ on calculated values for $n(\lambda)$ was investigated in four different ways. First, the SKK analysis was made with a straight line for $k(\lambda)$ between the ends of the solid-line curves at 22 Å and 1250 Å. At 400 nm this gave $n = 1.3558$ as compared with 1.343 from Irvine and Pollack¹ and at 2 μm , 1.2947 as compared with 1.304 and 1.302 from Irvine and Pollack¹ and Zolotarev *et al.*,² respectively. Second, the SKK analysis was made for $k = 1.55 \times 10^{-3}$ throughout the 50–1200-Å region and then a straight line joining $k = 1.55 \times 10^{-3}$ at 1200 Å to the end of the solid-line curve at 1250 Å. This gave $n = 1.336$ at 400 nm, and $n =$

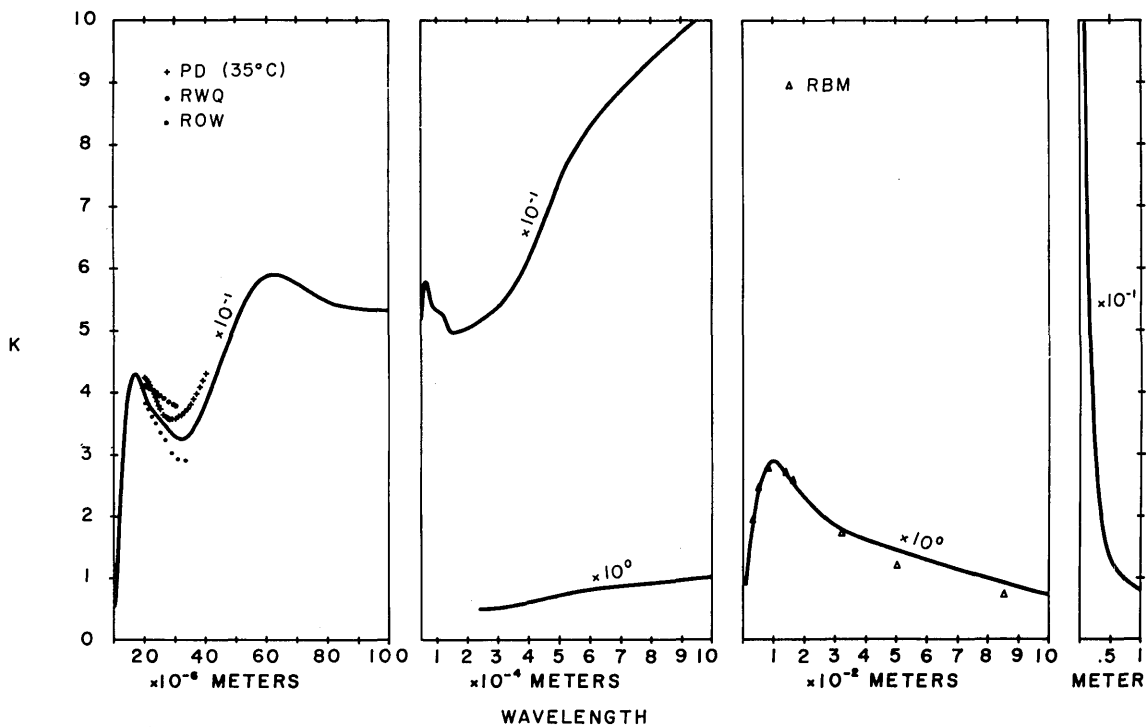


Fig. 5. Extinction coefficients of water for the 10^{-10} - μm spectral region. Notation and curves are described in the text.

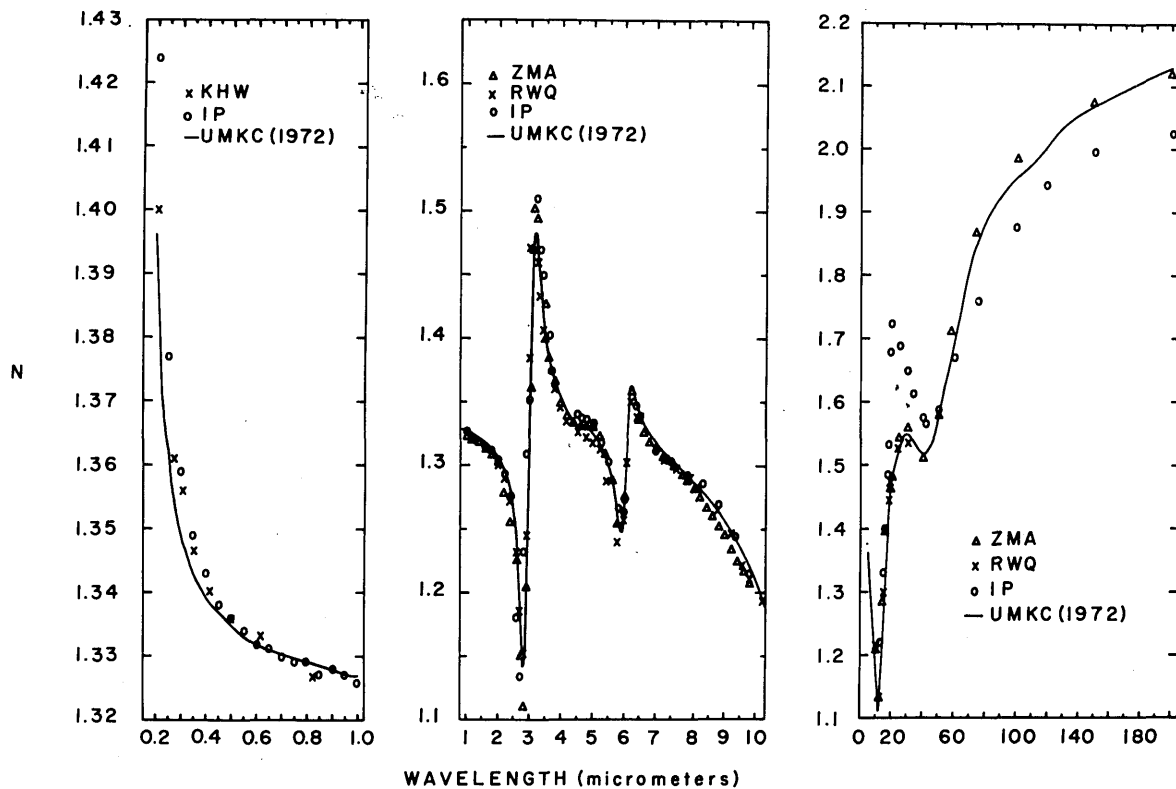


Fig. 6. Index of refraction of water for the spectral regions 0.2 - $200 \mu\text{m}$. Descriptions of the curves and the symbols are presented in the text.

1.309 at 2 μm . Third, the SKK analysis was made with the curve marked KHW joined smoothly to the dashed-line curve. This gave $n = 1.3449$ at 350 nm as compared with 1.349 from Irvine and Pollack.¹ Fourth, the effect of the amplitude of the curve for $k(\lambda)$ at about 880 Å was determined by raising only the peak value of the dashed-line curve to that for the KHW curve while other parts of the dashed-line curve remained fixed. This changed n at 200 nm from 1.3954 to 1.3957. Although these four tests indicate other postulated curves for $k(\lambda)$ could yield equivalent results, the final values for $n(\lambda)$ shown in Table I and Fig. 6 were obtained by applying the SKK analysis to the continuous curve described in Sec. III of this paper.

Values of $n(\lambda)$ from Refs. 1, 2, 5, and 8 are compared graphically in Fig. 6 with $n(\lambda)$ obtained during the present investigation. In the 0.2–0.6- μm region $n(\lambda)$ from the present work are less than those from Irvine and Pollack¹ (IP) and from Kerr *et al.*⁸ (KHW). In part this is attributed to the influence of the curve postulated for $k(\lambda)$ in the uv on results of the SKK analysis in the 0.2–0.6- μm region. Additional investigations of the height, width, shape, and number of vacuum-uv absorption bands are needed in the future in order to resolve these discrepancies. In the 1.0–6.0- μm region $n(\lambda)$ from IP and from Rusk *et al.*⁵ (RWQ) are slightly lower than $n(\lambda)$ determined during the present investigation. The maximum and minimum values of $n(\lambda)$ in the region of the water band centered at 2.95 μm are, respectively, less than and greater than values for similar quantities from IP and from Zolotarev *et al.*² (ZMA). Values of $n(\lambda)$ from ZMA and RWQ are in best agreement with $n(\lambda)$ from the present investigations in the regions 3.1–6.0 μm and 7.5–9.0 μm , respectively. Values of $n(\lambda)$ from Ref. 2 (ZMA) for the 10–200- μm region are in good general agreement while those from Ref. 1 (IP) do not agree with $n(\lambda)$ determined during the present investigations. We feel the values from Ref. 1 are in error in the long wavelength region.

We repeat the encouragement¹ that authors in the future present their data in tabular form because it was very difficult to accurately read many of the graphs.

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COMPUTERS IN CHEMICAL RESEARCH AND EDUCATION

An international conference will be held at Ljubljana and Zagreb, Yugoslavia, on 12-17 July 1973. The topics to be treated are theoretical chemistry, computer simulations of complex processes, computer designed synthesis, computer control of experiments, data acquisitions and refinement, analysis and simulations of complex spectra, structure determination from complex data, computer in teaching, computer assisted handling of chemical informations, communications, networks, and program exchange. Further details from D. Hadži, Boris Kidrič Institute, P.O. Box 380, 61001 Ljubljana, Yugoslavia.