

# **Equivalence of Kramers-Kronig and Fourier Transforms to Convert between Optical Dispersion and Optical Spectra**

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(Received May 14, 2012)

## **Abstract**

The complex refractive index relates optical dispersion, which describes the variation of refractive index with wavenumber, to the corresponding absorption spectrum; both phenomena are associated with the same underlying molecular property, electric dipolar moment. Instead of the traditional Kramers-Kronig transform for interconversion between absorption and dispersion, we show the practicality of Fourier transforms for this purpose, and prove the equivalence of these transforms. We demonstrate the transforms with infrared data for liquid benzene.

## **1 Introduction**

Optical absorption and its variation with wavenumber in a spectrum are much more commonly described and applied than refractive index and its analogous variation as dispersion; there exists little discussion of the practical relation between these phenomena. Our objective is to explain, on the basis of a mathematical analysis, both this relation and how these properties can be measured readily in a typical contemporary laboratory for instrumental analysis.

According to a novel approach, we explain how to derive both optical absorption and optical dispersion from measurements in a single set and with existing instruments.

We define pertinent quantities. For a pure substance in a gaseous, liquid or solid state of aggregation under specified conditions, the *refractive index* at a particular wave length is a fundamental physical property that has traditionally served for identification of a chemical compound, or for confirmation of its chemical purity, or as a measure of its concentration in a mixture. The refractive index  $n(\lambda)$  of a substance at wave length  $\lambda$  is an intensive and dimensionless quantity defined as the ratio of the speed  $c_0$  of light in vacuo to the speed (magnitude of phase velocity)  $c(\lambda)$  in the medium:

$$n(\lambda) = \frac{c_0}{c(\lambda)} \quad (1)$$

a phase velocity signifies the rate at which the crest of a wave form propagates. The variation of refractive index with wave length or frequency is called *optical dispersion*. Because electromagnetic frequency  $\nu$ , or preferably its quotient  $\frac{\nu}{c_0}$  called *wavenumber* (reciprocal of wave length  $\lambda$ ) and denoted with symbol  $\tilde{\nu}$ , is a quantity more meaningful than wave length in relation to the energies of molecular states, we work henceforth in terms of wavenumber.

A direct measure of absorption is *absorbance*  $A$ ,

$$A(\tilde{\nu}) = \log_{10} \left[ \frac{I_0(\tilde{\nu})}{I(\tilde{\nu})} \right] \quad (2)$$

which is a briggsian logarithmic ratio of intensity of light incident on a sample,  $I_0(\tilde{\nu})$ , and transmitted through it,  $I(\tilde{\nu})$ , at wavenumber  $\tilde{\nu}$ . For any real sample, the extent of absorption of light at a particular wavenumber, or the absorbance there, is proportional to the thickness of a sample or to the concentration of an absorbing substance within a path of fixed length. For a sample of concentration  $c$  (distinct from speed of light in a medium that shares the same symbol according to SI convention) of an absorbing substance and length  $l$  of optical path within which absorption occurs, a relation between absorbance,  $A(\tilde{\nu})$ , and concentration or length of optical path at a particular wavenumber, is

$$A(\tilde{\nu}) = \epsilon(\tilde{\nu}) c l \quad (3)$$

The factor of proportionality, *absorption coefficient*,  $\epsilon(\tilde{\nu})$ , is hence an intensive quantity but not dimensionless. A further necessary quantity is thus *absorption index*  $\kappa(\tilde{\nu})$ , related as follows to absorbance  $A(\tilde{\nu})$  of a pure isotropic film of thickness  $l$  at wavenumber  $\tilde{\nu}$ ,

$$\kappa(\tilde{\nu}) = \ln_e(10) \frac{A(\tilde{\nu})}{4\pi\tilde{\nu}l} \quad (4)$$

This absorption index is, like refractive index, both an intensive and dimensionless quantity. A significant distinction between absorption coefficient  $\epsilon(\tilde{\nu})$  and absorption index  $\kappa(\tilde{\nu})$  is the presence of wavenumber  $\tilde{\nu}$  in the latter denominator. As the absorption coefficient of a substance tends to increase with the wavenumber of a spectral transition from the far infrared to the xray regions, a wavenumber divisor to form the absorption index tends to moderate this effect.

Through recording and qualitatively interpreting nuclear-magnetic-resonance, infrared and ultraviolet spectra as part of their practical work in chemical laboratories, chemists become familiar with the principles of spectrometry underlying measurements from the radio-frequency region to the xray region and measured in absorption, emission, photoluminescence and Raman scattering modes. The *optical activity* of carbohydrates in their separate dextro, D, or laevo, L, configurations, according to which a solution of sucrose, for instance, rotates a plane of polarization of linearly polarized visible light, is well known; less well known is *optical rotatory dispersion*, according to which optical isomers of chiral compounds such as proteins exhibit signals of opposite sign in the ultraviolet region through values of refractive index that differ for left- and right-circularly polarised light. According to *circular dichroism*, these optically active compounds absorb, to slightly differing extents, left- and right-circularly polarized light in the same spectral region in which they exhibit optical rotatory dispersion. One might thus associate a rapid variation in refractive index with an absorption feature: between the latter properties there is an intimate link of a complex nature.

A measurement of the refractive index of a liquid organic chemical substance was formerly an essential activity in a characterization of that compound; for this reason handbooks of chemistry and physics list the refractive index of each compound. Chemists now make little direct use of that property, but one continuing application is for the detection of compounds separated in a liquid chromatograph. For such purposes, visible light is typically used, either with yellow light from a sodium lamp or with white light if compensating prisms are introduced into the optical path; the samples to which this technique is applied are typically transparent and colourless. Chemists might be unaware of a strong connexion between an absorption spectrum with discrete lines and the corresponding optical dispersion; in the visible spectral region, common liquid organic chemical substances are typically transparent, and the refractive index

generally varies little with frequency.

In contrast, in the mid infrared region, any organic chemical compound as a liquid sample shows spectral lines in absorption at wavenumbers in a sequence characteristic of the constitution of that compound, but chemists might fail to entertain an idea that the infrared dispersion has a correspondingly abundant pattern. The relation between absorption spectra and optical dispersion might form the basis of an experiment in the teaching of chemistry, although the limitations of commonly available instruments prove an impediment for this purpose in a traditional manner; on the basis of our mathematical derivation, we describe below a procedure to overcome this obstacle. Including this topic with infrared spectrometry would enable an acquisition of an increased appreciation of optical phenomena in relation to chemical applications, based on their inter- relation through various mathematical transforms.

The real refractive index is an optical property that measures the extent to which a ray of light is deflected angularly on passing from one medium into another. Even for a ray of light at normal incidence at a smooth interface between two media, that beam is partly reflected and partly refracted or transmitted, to an extent again depending on the refractive indices of the two media. The speed  $c_0$  of propagation of electromagnetic radiation in vacuo or empty space is constant independent of frequency, but in a medium the speed is typically smaller than  $c_0$  and varies with wave length. The real refractive index accordingly varies with wavenumber, and might even become less than unity, such as in the xray region. For an anisotropic sample, refractive index is a tensorial quantity: its magnitude depends on the direction of a light beam with respect to crystal axes.

When a real material is subjected to an electric field that is one component of electromagnetic radiation at any frequency, it becomes polarized, but such polarization is not an instantaneous response to that imposed field. A real material is, moreover, an imperfect insulator: an applied electric field induces a direct current proportional to the conductivity of that material; we ignore non-linear effects that occur under the influence of sufficiently large field strengths. In both cases these phenomena imply a dissipation of energy within a medium when light shines on a sample. To encompass these dissipative effects, in year 1895 Larmor [1] defined a *complex index of refraction*, introduced as follows.

## 2 Complex index of refraction

The purpose of recognizing a combination of two, distinct and real, physical quantities, separately observable, within a complex formula is to define quantitatively their inter-relation; optical absorption and optical dispersion are so inter-related. This formula for the complex index of refraction  $\eta(\tilde{\nu})$ ,

$$\eta(\tilde{\nu}) = n(\tilde{\nu}) + i \kappa(\tilde{\nu}) \tag{5}$$

relates real refractive index  $n$  and real absorption index  $\kappa$  at the same wavenumber  $\tilde{\nu}$ ;  $i = \sqrt{-1}$ . According to their appearance within the same formula, these quantities  $n(\tilde{\nu})$  and  $\kappa(\tilde{\nu})$  are hence not independent of each other. For the traditional conversion between these quantities, Kramers [2, 3] and Kronig [4] proposed these relations that constitute integral transforms,

$$n(\tilde{\nu}) - 1 = \frac{2}{\pi} \mathcal{P} \int_0^{\infty} \frac{\omega \kappa(\omega)}{\omega^2 - \tilde{\nu}^2} d\omega \tag{6}$$

$$\kappa(\tilde{\nu}) = -\frac{2\tilde{\nu}}{\pi} \mathcal{P} \int_0^{\infty} \frac{n(\omega) - 1}{\omega^2 - \tilde{\nu}^2} d\omega \tag{7}$$

which are actually Hilbert transforms [5,6], as discussed elsewhere [7]. For these improper integrals between end points 0 and  $\infty$ ,  $\mathcal{P}$  denotes that the Cauchy principal value is to be taken; a Cauchy principal value arises in an evaluation of an improper integral -- one with either  $0$  as lower limit or  $\infty$  as upper limit, or with a singularity within the interval between its end points. To avoid use of a compound symbol such as  $\tilde{\nu} \mp$  we simplify the notation for the purpose of these calculations with  $\omega$  as a formal integration variable of wavenumber type, not implying angular frequency. Kronig [4] derived equation 6 in a context of a theory of absorption and dispersion of xrays, but Kramers contended [2] that both relations have general applicability. In both equations, the number unity might be replaced by the value of the refractive index as  $\tilde{\nu} \rightarrow \infty$ .

In a region of wavenumber  $\tilde{\nu}$  in which occurs specific absorption by a chemical sample, so that  $A(\tilde{\nu})$  or  $\epsilon(\tilde{\nu})$  or  $\kappa(\tilde{\nu})$  is  $> 0$ , and with maximum absorption at  $\tilde{\nu}_0$ , real refractive index  $n(\tilde{\nu})$  varies rapidly with  $\tilde{\nu}$ , increasing from  $\tilde{\nu}$  less than  $\tilde{\nu}_0$  in what is regarded as *normal dispersion*. Just less than wavenumber  $\tilde{\nu}_0$ , a maximum, of value  $n_{\max}$ , occurs, followed by an abrupt decrease below the stable value beyond  $\tilde{\nu}_0$  to a minimum,  $n_{\min}$ , and then a gradual increase approaching that stable value, as illustrated at several points within figure 3

introduced below. Although that anomaly resembles the shape of a curve for the first derivative of absorbance with respect to wavenumber in that region, that derivative is a feature generally narrower than the corresponding dispersion feature. For an absorption line of lorentzian profile, of algebraic form shown below, a difference  $n_{\max} - n_{\min}$  is related to the maximum absorption index  $\kappa_0$  at wavenumber  $\tilde{\nu}_0$  [8].

### 3 Infrared spectrum of liquid benzene

As a vehicle to which to apply these relations, we simulate an absorption spectrum in the mid-infrared region as a sum of lorentzian terms, one term for each spectral line, according to this formula:

$$A(\tilde{\nu}) = \sum_{j=1} \frac{a_j b_j}{\pi [(\tilde{\nu} - \nu_j)^2 + b_j^2]} \quad (8)$$

This simulation is designed to reproduce an experimental spectrum, but lacks a complicating presence of noise, so as to facilitate the calculation of continuous Fourier transforms to follow. Each narrow spectral line in absorption is thus assumed to have a lorentzian profile according to a particular term in that sum;  $b_j$  denotes here half the width at half the maximum net absorption at wavenumber  $\tilde{\nu}_j$ . As the area under the curve defined by a single term pertaining to a single spectral feature without multiplicand  $a_j$  is unity, parameter  $a_j$  defines the relative total or integrated intensity of each various contribution to the absorption spectrum.

For the first nine decades during which spectra were recorded in the mid-infrared region, almost all instruments for this purpose were spectrometers in which a salt prism or a reflective diffraction grating, or both, dispersed radiation from an incandescent source into more or less narrow bands at variable wavenumbers at which absorption was measured in a sequential manner. The conversion between absorption and dispersion phenomena was customarily effected through the Kramers-Kronig transforms in formulae 6 and 7. In contrast, a contemporary chemical laboratory typically contains a non-dispersive instrument to produce infrared spectra. Its essential optical element is an interferometer, commonly of Michelson's design [9, 10]; the intensity  $I(l)$  of transmitted light therein is measured as a function of difference  $l$  of lengths of paths between two divided beams formed with a beam splitter and appropriate mirrors. The interferogram directly measured is conventionally converted to chemically meaningful data through a Fourier transformation. In what follows we describe a

new procedure to derive both an absorption spectrum and the corresponding optical dispersion from the same sample and from measurements in a single sequence.

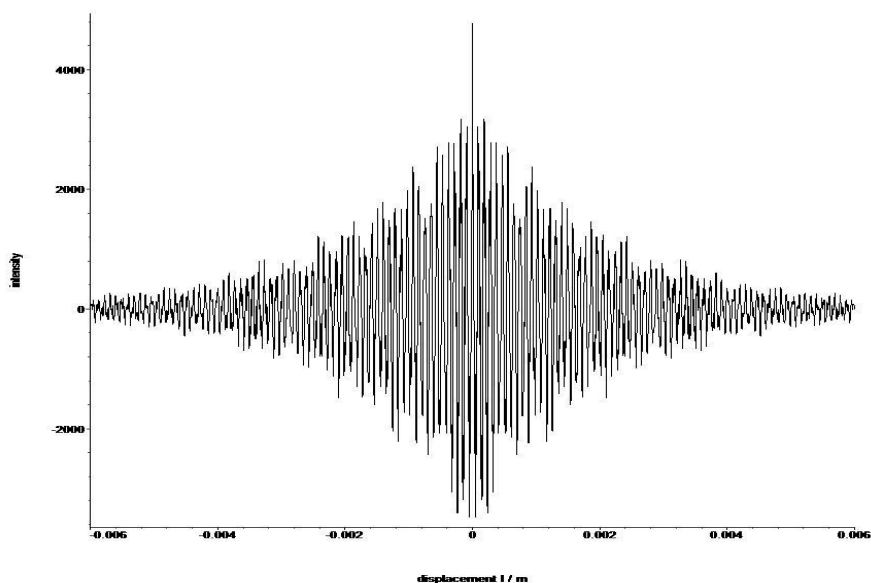
By means of such an interferometer, the intensity contributed from radiation within a pertinent domain of wavenumber is measured at all times; the spectrum displayed as absorbance,  $A(\tilde{\nu})$ , as a function of wavenumber is calculated from that interferogram  $I(l)$  by means of a *Fourier transform* or *exponential transform*.

$$A(\tilde{\nu}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} I(l) \exp(-i\tilde{\nu}l) dl \quad (9)$$

Integration should be made, in principle, over displacements  $l$  between  $-\infty$  and  $\infty$ , but, because the pattern of intensity decays exponentially in both directions from the zero path difference, at  $l = 0$ , the calculation with a path difference over a finite domain including the zero value suffices for practical purposes. The spectral resolution is limited by the maximum path difference; for a maximum path difference 0.01 m, the spectral resolution is accordingly  $\sim 100 \text{ m}^{-1}$ . Figure 1 presents an interferogram for pure liquid benzene simulated as a sum of terms,

$$I(l) = \sum_j a_j \cos(\tilde{\nu}_j l - b_j |l|) \quad (10)$$

in which quantities  $a_j$ ,  $b_j$  and  $\tilde{\nu}_j$  have the same significance as in formula 8 above. To generate this particular interferogram, we fitted, with lorentzian profiles, lines in an experimental spectrum of liquid benzene, for a sample of thickness  $(5.0 \pm 0.2) \times 10^{-6}$  m, and collected the parameters to define the eight most intense absorption features characterized by wavenumber  $\tilde{\nu}_j$  between  $20000 \text{ m}^{-1}$  and  $400000 \text{ m}^{-1}$ ; other absorption features are negligible for the present purpose. Any real spectrum of a particular sample in absorption is, however, measured not directly, but rather as a ratio between a background spectrum, of which the complicated curve of the spectral profile depends on the characteristics of the source, detector and other components between source and detector without a sample, and a spectrum of that sample, which contains, in addition to features in the background curve, absorption lines due to the sample compound. An interferogram of a particular sample is thus measured indirectly as it includes the effects of source, detector and other



**Figure 1** Interferogram of intensity  $I(l)$  vs displacement  $l$  of an interferometer, simulated for infrared absorption of liquid benzene

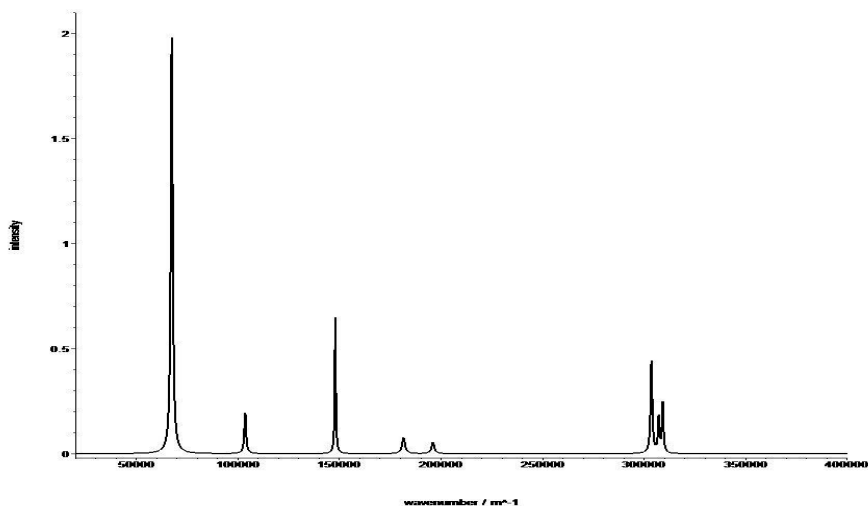
components between these optical elements apart from the sample; these experimental aspects are neglected in our analysis here as they are incidental to the mathematical methods, physical principles and chemical applications. Through our simulations, we avoid distraction from other experimental effects [9, 10] such as phase errors, truncation errors, apodization perturbations and non-lorentzian line shapes that are likewise incidental to the physical principles and mathematical analysis.

Direct application of the *Fourier exponential transform*, according to formula 9, to the simulated interferogram  $I(l)$  in figure 1 generates directly a corresponding spectrum as absorbance  $A(\tilde{\nu})$  versus wavenumber  $\tilde{\nu}$  in figure 2. A *Fourier cosine transform* of that interferogram  $I(l)$ ,

$$\sqrt{\frac{2}{\pi}} \int_0^{\infty} I(l) \cos(l\tilde{\nu}) dl \quad (11)$$

generates *exactly the same spectrum* as in figure 2, so again the curve of  $A(\tilde{\nu})$ . Specifying 0 and





**Figure 2** Infrared spectrum of liquid benzene calculated from either a Fourier exponential transform or a Fourier cosine transform of the interferogram in Figure 1

$\infty$  as bounds for a domain of this integral, we take advantage of the symmetry of the interferogram: the pattern in figure 1 is a rigorously even function, such that  $I(l) = I(-l)$ ; with a factor 2, we replace the doubly infinite range of integration in formula 9 with a singly infinite range in formula 11. These spectra from the Fourier exponential transform and the Fourier cosine transform of the same interferogram are identical for the following reason. We express the exponential factor  $\exp(-i\vec{l}\vec{\nu})$  in the Fourier transform in trigonometric form according to Euler's identity.

$$\exp(-i\vec{l}\vec{\nu}) = \cos(\vec{l}\vec{\nu}) + i \sin(\vec{l}\vec{\nu}) \quad (12)$$

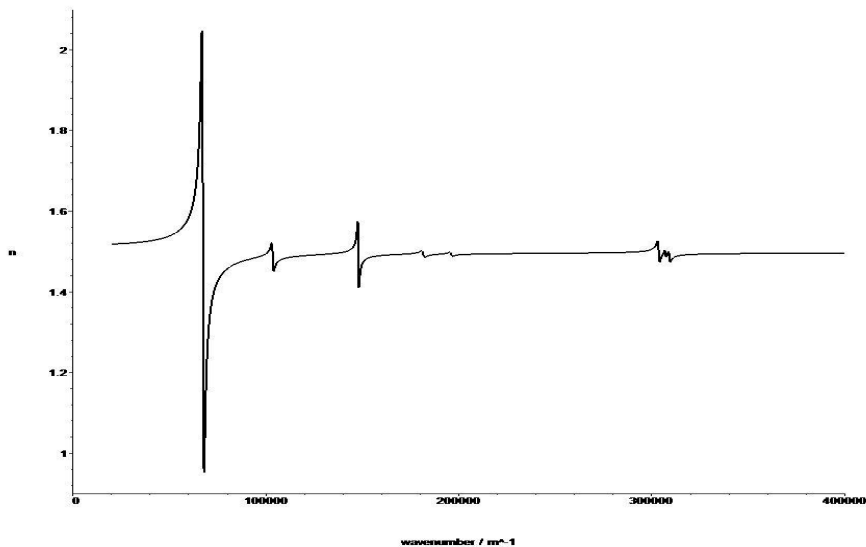
Because formula 10 is by design an even function, as shown in figure 1, there is rigorously no contribution to that Fourier exponential integral over the integration range  $-\infty$  to  $\infty$  from the sine term in the imaginary part on the right side of equation 12.

#### 4 Infrared dispersion of liquid benzene

For the same reason, the *Fourier sine transform* integrated over a doubly infinite range,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} I(l) \sin(\vec{l}\vec{\nu}) dl \quad (13)$$

is zero, but integration between end points 0 and  $\infty$  yields a non-zero result; that curve, shifted



**Figure 3** Infrared dispersion of liquid benzene calculated either from a Fourier sine transform of the interferogram in figure 1 or from a Kramers-Kronig transform of the spectrum in figure 2, in both cases taking account of the sample thickness and a wavenumber factor; this curve is practically indistinguishable from a variation of refractive index directly measured in the mid infrared region.

upward 1.478 units to reproduce the refractive index  $n_D$  of benzene at 589.3 nm, resembles the infrared dispersion of liquid benzene. When we apply a Kramers-Kronig transformation, formula

6, to the formula of the curve plotted in figure 2 as the absorption spectrum, with the same shift upward we obtain a curve *indistinguishable* from that obtained directly from the Fourier sine transform. In both cases the result merely *resembles* the variation of refractive index with wavenumber  $\tilde{\nu}$  across the mid infrared region. The distinction between the curve from that transform of the absorption coefficient and the true infrared dispersion arises because absorption coefficient  $\epsilon(\tilde{\nu})$  differs from absorption index  $\kappa(\tilde{\nu})$ , defined through formula 4.

When absorbance or absorption coefficient is converted to absorption index, each as a function of wavenumber, such as with formula 4, a Kramers-Kronig transformation of the resulting curve yields, with the same shift +1.478 units, directly the infrared dispersion curve in figure 3 that is quantitatively consistent with experiment [11, 12,13]. The curve from the Fourier

sine transform of the interferogram, analogously adjusted with the coefficient of  $A(\tilde{\nu})$  in the right side of equation 4, generates a curve indistinguishable from that from the Kramers-Kronig transformation, hence likewise the infrared dispersion. Our appendix proves that these transformations are equivalent.

Our analysis here signifies that an application to an absorption spectrum of an *inverse Fourier cosine transform*, of which the form is identical to that of a direct Fourier cosine transform in formula 10, yields an interferogram; the Fourier sine transform of that interferogram yields a curve from which the optical dispersion is obtained on taking into account the thickness of the sample and a wavenumber factor. The reverse conversion of a curve for optical dispersion into an absorption spectrum is equally verified. This result is hence consistent with our observation that an explicit application of a Fourier sine transform to an interferogram recorded with a Michelson interferometer in the customary manner yields directly, on taking into account the thickness of the sample and a wavenumber factor, a curve depicting the variation of refractive index with wavenumber.

It is known [9], although seldom practised, that placing a sample in one arm of a Michelson interferometer enables one to derive that dispersion  $n(\tilde{\nu})-1$ , but manufacturers of commercial interferometric instruments generally fail to cater for such measurements in their instrumental designs; such a condition inhibits experiments on this topic in instrumental analysis and physical chemistry. Our above derivation demonstrates that a sample placed in a common optical path, such as at a conventional sample position, can, however, yield the dispersion, simply on performing a *Fourier sine transform* of the recorded interferogram instead of a *Fourier exponential transform* or *Fourier cosine transform*, and on taking into account the thickness of the sample and wavenumber factor  $\tilde{\nu}$ . When the resolution of an infrared interferometric spectrometer is comparable with, or greater than, the width of an absorption line, that line might be measured more accurately through the infrared dispersion than through the absorption, because the dispersion feature is typically wider than the absorption feature, and thus less susceptible to instrumental distortion due to inadequate resolution. Moreover, the relation that a difference  $n_{\max} - n_{\min}$  equals, for a lorentzian profile that an absorption line of a liquid sample commonly approximates, a maximum value  $\kappa_0$  of the absorption index, might increase the accuracy of a determination of intensity, and hence of a thickness or concentration of a sample. Although, in principle, a full Fourier exponential transform of an interferogram to yield a spectrum, followed by a Kramers-Kronig transform in formula 6 applied to that

spectrum, with an appropriate wavenumber factor  $\bar{\nu}$ , produces the same dispersion, the propagation of inevitable noise at the detector of radiation in the interferometer might make these two operations susceptible to greater error in an eventual dispersion curve than from a single operation comprising the sine transform of an interferogram [8]. Despite a view, expressed about the Kramers-Kronig relations relating dispersion and absorption, that there exists a "general lack of confidence in their strict validity" [15], the application of a Fourier sine transform, and of also a Fourier cosine transform if necessary, both confirms the validity of these relations and makes them superfluous. A *Maple* worksheet illustrating the present phenomena is included in part II of a book [16] to appear shortly.

## 5 Discussion and conclusion

The derivation in the appendix and associated relations were discovered independently by the authors in a spirit of experimental and constructive mathematics applied to spectral phenomena with significant chemical application, because symbolic computation with a contemporary processor provides not only a valuable medium to teach and to learn mathematics but also an excellent tool to explore the mathematical aspects of chemical and physical phenomena. Much of the above content was, nevertheless, known; Bertie and Zhang [14] stated "the infinite Kramers-Kronig transform is equivalent to the infinite Hilbert transform, which is equivalent to the allied Fourier integrals". Despite that assertion, these relations are poorly known to practitioners of infrared interferometric spectrometry, as attested by their absence from recent and otherwise authoritative monographs [9, 10]. Bertie and Zhang included in their article [14] a listing of a subroutine (140 lines of *Fortran 77* code) for a rapid discrete Kramers-Kronig transform; both our continuous Kramers-Kronig transforms and Fourier exponential, sine and cosine transforms were each accomplished with one, simple, *Maple* command that is a direct implementation of an algebraic formula as stated above; the corresponding integral has explicit end points 0 or  $-\infty$  and  $\infty$  as appropriate, requiring only a few seconds for execution on a typical computer.

We here demonstrate the link between an absorption spectrum and optical dispersion in the same spectral region; a reader can hence appreciate the existence of a connexion between an excited state of discrete energy, to which a transition occurs from the ground state on absorption of a photon, and the variation of refractive index at wavenumbers corresponding to the same energy difference. Both absorption and refractive indices manifest properties of the molecular

electric dipolar moment that are irrelevant here. It is important to be aware of optical dispersion because the reflectance spectrum, and even the absorption spectrum of samples under various conditions, can include a component of dispersion; the measured spectrum is then a sum of absorption and dispersion to varied extents [10]. Beyond elucidating the nature of absorption spectra and the related variation of refractive index with wavenumber, which our computational experiment shows to convey equivalent information, our discussion demonstrates that it is important for complex variables to be included within the mathematical experience of chemists.

*Acknowledgements:* We thank Dr. C. D. Keefe for providing an infrared absorption spectrum of liquid benzene and Professor J. E. Bertie for providing pertinent documents.

## Appendix: Derivation of the Kramers-Kronig transform from Fourier transforms

To understand the equivalence of these transforms, we report the following original derivation. For an integral that effects an inverse Fourier cosine transform of function  $\kappa(\tilde{\nu})$  to generate an interferogram  $I(l)$ ,

$$\sqrt{\frac{2}{\pi}} \int_0^{\infty} \kappa(\tilde{\nu}) \cos(l\tilde{\nu}) d\tilde{\nu} \quad (14)$$

we defer that integration and transfer the integrand and external factor  $\sqrt{\frac{2}{\pi}}$ , with  $\omega$  replacing  $\tilde{\nu}$  in  $\kappa(\tilde{\nu})$  because it eventually becomes integrated over, into an improper integral for a Fourier sine transform,

$$\sqrt{\frac{2}{\pi}} \int_0^{\infty} \left[ \sqrt{\frac{2}{\pi}} \kappa(\omega) \cos(l\tilde{\nu}) \right] \sin(l\omega) dl \quad (15)$$

Here  $\omega$  in  $\sin(l\omega)$  is the same dummy integration variable of wavenumber type. We assume that  $\kappa(\omega)$  is a function well behaved such that  $I(l)$  tends to zero as  $l \rightarrow \infty$ , in which case the integral evaluates to zero at that upper limit of the corresponding improper integral; we then evaluate the result at the lower end point  $l = 0$ , which after trivial algebra yields this result:

$$-\frac{2}{\pi} \frac{\omega \kappa(\tilde{\nu})}{\tilde{\nu}^2 - \omega^2} \quad (16)$$

On imposing formally thereon the deferred integration over  $\tilde{\nu}$ , which corresponds to merely altering the order of integration in the implied double integral, we obtain

$$\frac{2}{\pi} \int_0^{\infty} \frac{\omega \kappa(\omega)}{\omega^2 - \tilde{\nu}^2} d\tilde{\nu} \quad (17)$$

which is exactly the right side of the Kramers-Kronig relation, equation 6, with  $n(\bar{\nu})-1$  on the left side.

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