TABLE III

Percent Discount or Premium for Green Grade, Refining Loss, and Refined Bleached Color of Green Soybean Oils

Oil	Green-grade discount	Discount for RBC[a]	Discount or premium for RL[b]	Net discount
1954 Beans				
5	1	Sample grade	1.80 (discount)	Sample grade
6	1	None[c]	0.22 (premium)	0.78
7	1	None[c]	0.07 (premium)	0.93
9	2	6.25[c]	2.25 (discount)	8.50
1952 Beans				
5	1	Sample grade	0.22 (premium)	Sample grade
6	1	Sample grade	9.15 (discount)	Sample grade
7	1	Sample grade	6.45 (discount)	Sample grade
8	2	Sample grade	1.28 (discount)	Sample grade
9	2	Sample grade	12.00 (discount)	Sample grade

[a] RBC—refined bleached color.
[b] RL—refining loss.
[c] Green-grade discount applies only if RBC discount is less than green-grade discount.

blending frost- or drought-damaged soybeans with sound soybeans before processing has made it extremely difficult to procure samples of damaged soybeans or oil from damaged soybeans. Extensive green damage would raise processing problems in which the present N.S.P.A. grading system would not give the real value of the oil.

The authors are not in a position to state what effect variety, locality, and weather during the growing season may have had on the refining and bleaching qualities of the oil in frosted soybeans. There were however some indications that variety and processing were involved. Some samples of soybeans did not look unusually bad, but they produced dark oil whereas other soybeans which were entirely green and badly shriveled produced better oil.

Summary

Frosted soybeans and oils from frost-damaged soybeans were obtained from the farm and commercial sources. All soybeans used were classed as inferior, according to the Handbook of Official Grain Standards of the United States, with respect to both green and weather damage. Localities represented were Oklahoma, Mississippi, Illinois, and Iowa. Spectrophotometric measurements and visual comparisons were made to establish the green grades. If the necessary quantities of oils were available, the samples were refined and bleached; otherwise only the chemical analyses, green grading, and spectrophotometric measurements were made on the crude oils. Iodine values and free fatty acid were determined also.

If a spectrophotometric method for the green grading of soybean oil were to be adopted, present indications are that the boundary between grades 1 and 2, comparable to the present N.S.P.A. grading system, should be at optical density 0.45 at 700 mμ, as measured in a 21.8 mm. I.D. tube in a Coleman Model 6B instrument, and that between grades 2 and 3 should be at optical density 0.58. It is recommended that duplicate systems of green grading be avoided.

Acknowledgments

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The Infrared Spectra of Mono-, Di-, and Triglycerides[1]

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A RAPIDLY growing interest in various types of modified glycerides has been evidenced by an increasing number of publications describing their preparation, purification, physical and chemical properties, and their possible uses. These modified glycerides include products obtained by hydrogenation and fractionation, mixed glycerides of long- and short-chain fatty acids such as acetostearins, and mixtures of mono-, di-, and triglycerides.

While chemical methods for analyzing modified glycerides are generally satisfactory, some of them are tedious and others are not entirely adequate for investigational and control purposes. Physical methods which would provide rapid and convenient means of determining qualitatively and quantitatively specific glycerides present in admixtures as well as trans-isomer content would be extremely useful.

Infrared absorption appears to be a most promising physical tool for analytical purposes. However before development of any specific procedure can be attempted, the spectra of several pure glycerides, representative of the various types, must be obtained and characterized. Availability of such compounds in this laboratory has afforded an unusual opportunity to obtain and examine the infrared spectra of several types of glycerides. The purpose of this paper is to report the infrared spectra of 21 pure glycerides, including various mono-, di-, and triglycerides of long-chain (C_{14}, C_{16}, and C_{18}) fatty acids, both saturated and unsaturated, and of mixed long- and short-chain fatty acids, such as diacetotriglycerides. With two or three exceptions, which are included for completeness, none of these spectra has heretofore been published. The infrared spectra of these compounds in the rock salt region, 2 to 12 microns, are presented. Conclusions which can be obtained from their examination and which are of possible importance to the development of analytical methods are discussed.

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Experimental

Infrared absorption spectra were measured with a Model IR-2T Beckman Automatic Recording Infrared Spectrophotometer.[3] The instrument was housed in a room maintained at approximately 23°C. and

TABLE I

Source, Preparation, and Properties of Glycerides

Glyceride	Preparation and Properties
Tristearin	(2)
Tripalmitin	From pure palmitic acid esterified with glycerol. Tripalmitin obtained by repeated fractional crystallizations from solvents.
Triolein	From esterification of oleic acid with glycerol. Contains traces of tripalmitin and infrared absorption evidence of trielaidin (7).
Trielaidin	(8)
1,3-Distearin	From trityl glycerol and stearoyl chloride (23).
1,3-Dipalmitin	(9)
1,3-Diolein	Pure methyl ester interesterified with glycerol. Diolein separated by molecular distillation and fractional crystallization from solvents.
1-Aceto-3-stearin	(24)
1-Monostearin	(17)
1-Monopalmitin	From methyl palmitate and glycerol. Mixed palmitins molecularly distilled. First cuts combined and recrystallized from isopropanol. Filtrate recrystallized from hexane. Monopalmitin recovered from first crop. m.p. 70-77°C., theory 77°C. O–H 9.68%, theory 10.29%.
1-Monoolein	(6)
1-Monomyristin	Prepared by method similar to homolog monostearin (17).
Triacetin	Heart cut from Eastman Commercial Product[3] obtained from Distillation Products Industries, Rochester 3, N. Y. m.p. 154-155°C. at 22-23 mm. Hg. $n^{25°} = 1.4295$.
1,2-Diaceto-3-stearin	(24)
1,2-Diaceto-3-palmitin	By method for homolog, 1,2-diaceto-3-stearin (24).
1,2-Diaceto-3-olein	(6)
Tributyrin	Eastman Grade[3] obtained from Distillation Products Industries, Rochester 3, N. Y. Further purified by distillation and and crystallization.
1,2-Dibutyro-3-stearin	By method for homolog, 1,2-diaceto-3-stearin (24).
1,2-Dibutyro-3-palmitin	By method for homolog, 1,2-diaceto-3-stearin (24).
1,2-Dibutyro-3-olein	(6)
1,3-Dipalmito-2-lactin	(9)

20% relative humidity. The temperature of the spectrophotometer was maintained constant at 25°C. ± 0.1°C. by water circulated from a constant temperature bath. All samples were measured in chloroform solution against dry pure chloroform (22). Concentrations of the glycerides in the chloroform solutions were in all cases very close to 40 g. per liter. All measurements were made with the same 0.4 mm. rock salt cell.

All spectroscopic terms and symbols used throughout this paper are in conformity with the suggested nomenclature of the Joint Committee on Nomenclature in Applied Spectroscopy (10).

The preparation, purification, and physical and chemical properties of several of these compounds have been previously described, as indicated by the references in Table I. The source, purification procedure, and some pertinent physical constants for those compounds which have not heretofore been reported are included in the same table.

Infrared Absorption

The infrared spectra of the glycerides are shown in Figures 1, 2, 3, and 4. The prominent bands in these spectra are indicated in Figures 5 and 6. A cursory examination of these spectra reveals some half-dozen very prominent absorption bands common to the spectra of all compounds. These absorption bands arise from more or less well-known vibrations, as listed in Table II. As these bands are common to the spectra of all glycerides, they are of no value in the analysis of admixtures.

A more detailed study of the spectra (Figures 1-4) or of the charts (Figures 5 and 6) shows that absorption in three regions, in particular, might be useful to the development of analytical procedures. These regions are: a) the O–H stretching vibration at about 3 microns, b) the C–O stretching vibrations above 9 microns, and c) the C–H bending about the trans C=C groups above 10 microns.

[3]Mention of names of firms or trade products does not imply that they are endorsed or recommended by the U. S. Department of Agriculture over other firms or similar products not mentioned.

TABLE II

Most Prominent Absorption Bands in the Infrared Spectra of All Mono-, Di-, and Triglycerides

Wavelength position of maximum (microns)	Intensity	Most probable assignment
3.30–3.37	Very strong	C—H stretching (CH_3 and CH_2)
5.71–5.77	Very strong	C=O stretching (COOR)
6.83–6.88	Strong	C—H bending (doubly degenerate deformation of CH_3 and symmetrical deformation of CH_2)
7.23–7.35	Strong	C—H bending (symmetrical deformation of CH_3)
7.93–8.00	Strong	C—H in-plane wagging or rocking of CH_2 groups
8.48–8.58	Very strong	C—O stretching (COOR)

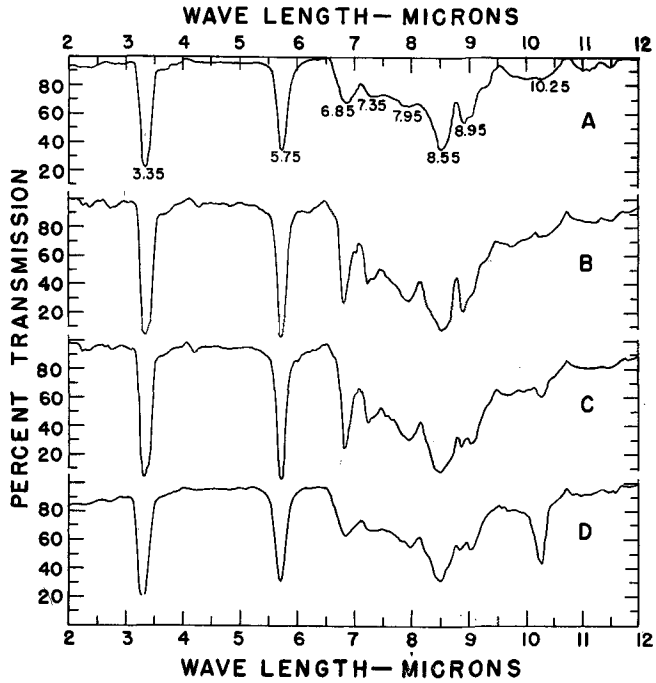

FIG. 1. Infrared absorption spectra of
A. Tristearin
B. Tripalmitin
C. Triolein
D. Trielaiden

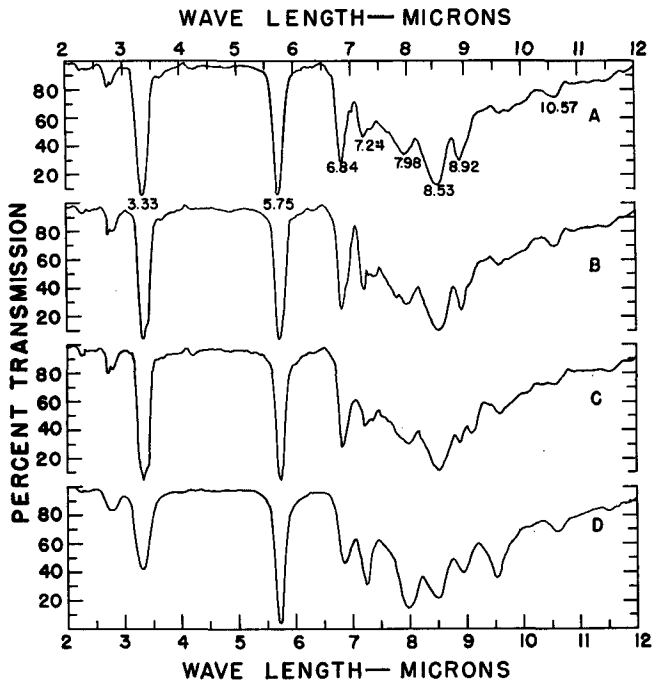

FIG. 2. Infrared absorption spectra of
A. 1-3 Distearin
B. 1-3 Dipalmitin
C. 1-3 Diolein
D. 1-Aceto-3-stearin

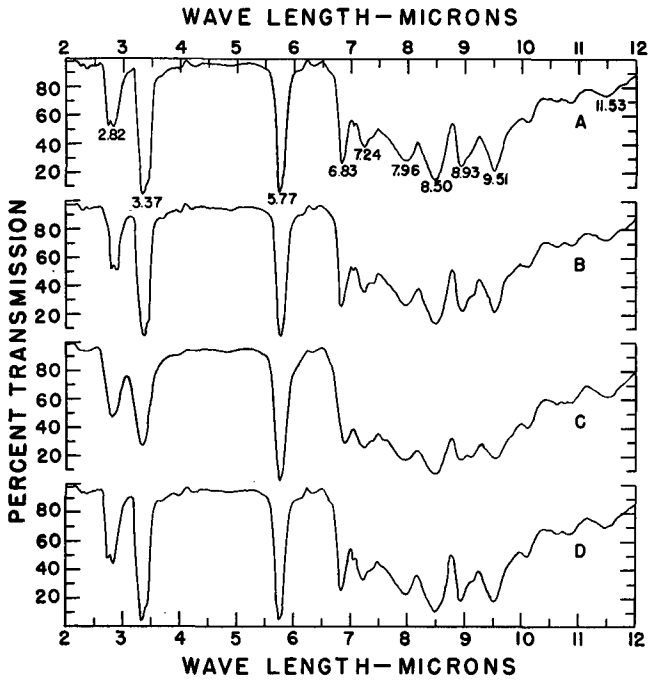

FIG. 3. Infrared absorption spectra of
A. 1-Monostearin
B. 1-Monopalmitin
C. 1-Monoolein
D. 1-Monomyristin

The 3.0 micron—O–H stretching vibration. Two bands with maxima at about 2.7 and 2.8 microns are found in this region (Table III). The combined intensities of these bands are considerably greater in the spectra of the monoglycerides than in those of the diglycerides, and they are completely absent in the spectra of triglycerides. The 2.7 micron band arises from a stretching vibration of a free O–H group. According to Smith and Creitz (18), the 2.8-micron band most probably arises from an O–H stretching vibration of the single bridged dimer. The stretching vibration of more highly hydrogen bonded O–H is masked by the strong C–H stretching vibration at 3.3 microns.

Observations of the infrared spectra of a triglyceride at these wave-lengths provide a ready check as to the presence of any mono- or diglyceride impurity. For example, in the preparation of diacetostearin from monostearin and acetyl chloride, the spectra of the purified triglyceride can be used to verify the complete absence of the original monostearin.

It would not be possible, from measurements in the 3-micron region, to determine whether or not the impurity in a triglyceride was a mono- or a diglyceride. Nor could the presence of monoglyceride in diglyceride, or conversely the presence of diglyceride in a monoglyceride, be detected. Fortunately, as will be shown, it does seem possible to make these distinctions in the region of C–O stretching.

Determination of mono- or diglycerides in triglycerides by use of the bands, about 3.0 microns, is limited to the analysis of triglycerides which do not contain hydroxy groups. Hydroxy-containing triglycerides cannot be analyzed by this method. This fact is illustrated by the last entry in Table III. Dipalmitolactin exhibits a spectrum with bands at 2.75 and 2.83 microns, resembling very closely the spectra of typical diglycerides. These bands arise obviously from O–H stretchings of the hydroxy group in the lactic acid portion of the molecule.

The 9.0 micron—C–O stretching vibrations. All long-chain glycerides exhibit bands at 8.9 and 9.1 mi-

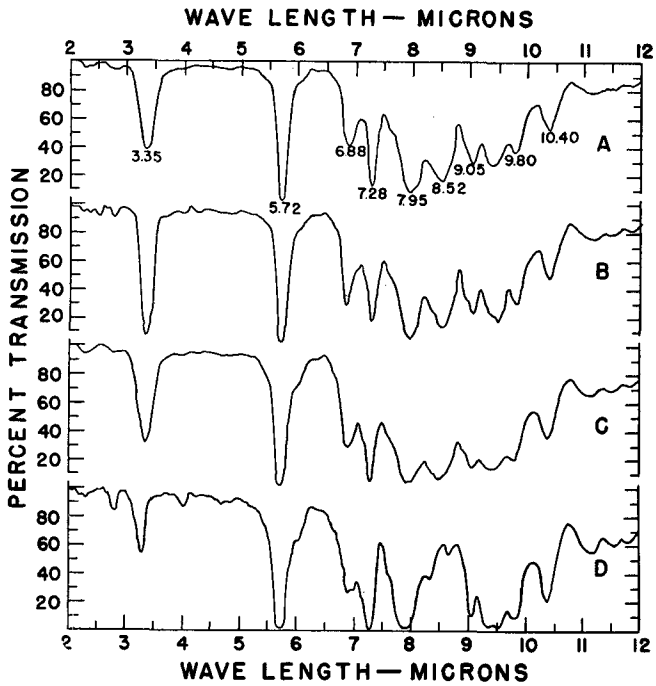

FIG. 4. Infrared absorption spectra of
A. 1,2-Diaceto-3-stearin
B. 1,2-Diaceto-3-palmitin
C. 1,2-Diaceto-3-olein
D. Triacetin

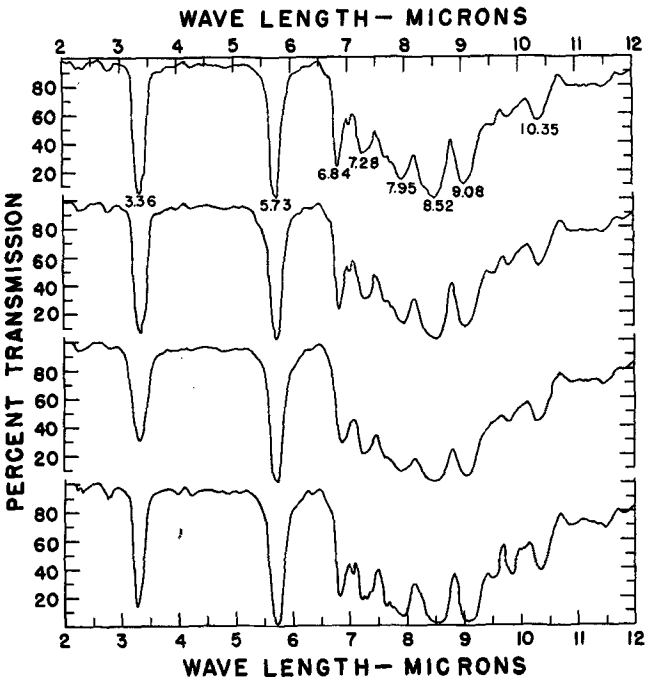

FIG. 5. Infrared absorption spectra of
A. 1,2-Dibutyro-3-stearin
B. 1,2-Dibutyro-3-palmitin
C. 1,2-Dibutyro-3-olein
D. Tri-n-butyrin

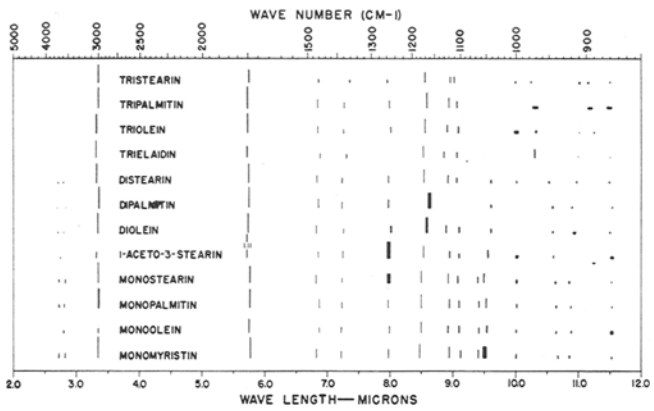

FIG. 6. Prominent absorption bands (wavelength position of maxima and intensities) in the infrared spectra of long-chain fatty acid glycerides.

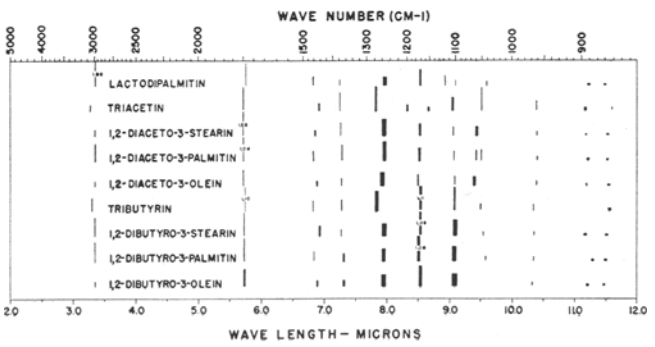

FIG. 7. Prominent absorption bands (wavelength position of maxima and intensities) in the infrared spectra of mixed long- and short-chain fatty acid glycerides.

TABLE III

The 3.0-Micron Band Arising from Free O–H Stretching Vibration

Glyceride	[a] 2.72–2.75μ	[a] 2.80–2.83μ
Tristearin	.....	.....
Tripalmitin	.....	.....
Triolein	.....	.....
Trielaidin	.....	.....
1,3-Distearin	0.060	0.052
1,3-Dipalmitin	0.069	0.061
1,3-Diolein	0.060	0.052
1-Aceto-3-stearin	0.064	.....
1-Monostearin	0.018	0.18
1-Monopalmitin	0.018	0.19
1-Monoolein	.....	0.14
1-Monomyristin	0.020	0.22
Triacetin	.....	.....
1,2-Diaceto-3-stearin	.....	.....
1,2-Diaceto-3-palmitin	.....	.....
1,2-Diaceto-3-olein	.....	.....
Tributyrin	.....	.....
1,2-Dibutyro-3-stearin	.....	.....
1,2-Dibutyro-3-palmitin	.....	.....
1,2-Diaceto-3-olein	.....	.....
1,3-Dipalmitito-2-lactin	0.078	0.067

crons, as shown in Table IV. The weaker band at 8.9 microns is not observed in the spectra of the mixed short- and long-chain glycerides (Table IV).

The region above 8 microns in the rock salt infrared absorption spectra has been referred to as the "fingerprint" region. Unlike the "group frequency" region below 8 microns (where most absorption bands can be assigned with some degree of certainty to vibrations of relatively simple groups which give rise to them), the "fingerprint" region exhibits bands that are more likely to arise from vibrations of larger groups and are often characteristic of the vibrating molecule as a whole. Hence less study has been made, in this region, attempting to correlate observed maxima with vibrating groups.

Bands about the region 8.9 to 9.1 microns have been assigned to the C–O stretching vibration of the C–O–C ether group (3, 4) and probably arise in these compounds from stretching vibrations in the C–O–C portion of the COOR ester group. This group would give rise to two C–O stretching vibrations, $R–C^{1}–O_{2}–C(=O)–$, (1) differing in frequency from (2) by reason of the unsaturated nature of the carbon atom (20, 21).

Kuhrt *et al.* (13, 14) have recently proposed the use of infrared spectra to detect the presence of monoglycerides in natural products by direct "fingerprint" comparisons of their spectra. These authors assign the bands at 8.9 and 9.1 microns as a doublet arising

TABLE IV

Absorption Bands in the Region of C–O Stretching and C–OH Bending — 9μ

Glyceride	Intensity at maxima				
	8.9μ	9.1μ	9.4μ	9.5μ	9.6μ
Tristearin	0.298	0.272	.....	.....	.....
Tripalmitin	0.407	0.306	.....	.....	.....
Triolein	0.327	0.312	.....	.....	.....
Trielaidin	0.251	0.244	.....	.....	.....
1,3-Distearin	0.345	0.244	.....	.....	0.133
1,3-Dipalmitin	0.381	0.228	.....	.....	0.156
1,3-Diolein	0.232	0.270	.....	.....	0.142
1-Aceto-3-stearin	0.313	0.243	.....	.....	0.350
1-Monostearin	0.376	0.309	0.297	0.412	.....
1-Monopalmitin	0.405	0.304	0.308	0.421	.....
1-Monoolein	0.319	0.304	0.258	0.304	.....
1-Monomyristin	0.460	0.312	0.354	0.472	.....
1-3-Dipalmito-2-lactin	0.341	0.238	.....	.....	0.172
Triacetin	.....	0.539	0.862	0.920	.....
1,2-Diacetostearin	.....	0.347	0.351	.....	.....
1,2-Diacetopalmitin	.....	0.388	0.406	0.464	.....
1,2-Diacetoolein	.....	0.339	0.338	.....	.....
Tributyrin	.....	0.952	.....	0.298	.....
1,2-Dibutyrostearin	.....	0.564	0.172	.....	.....
1,2-Dibutyropalmitin	.....	0.585	.....	0.196	.....
1,2-Dibutyroolein	.....	0.525	.....	.....	.....

from C–O stretchings of secondary alcohols. As the bands are observed in all spectra, even those of triglycerides, this correlation cannot be entirely correct.

Weniger in 1910 (25), early in the history of the application of infrared absorption to structural problems, noted that the position of this C–O band in the spectra of alcohols depended upon the primary, secondary, or tertiary character of the hydroxylated carbon atom. From this observation the inference has been drawn that primary, secondary, and tertiary alcohols can be distinguished by the appearance of characteristic absorption bands at 9.6, 9.1, and 8.6 microns, respectively. More recent studies have shown that this inference is not valid. Zeiss and Tsutsui (26) have demonstrated that substitution on the carbon atom, alpha to the hydroxylated carbon, will produce a considerable shift of band maxima to lower frequencies and cause considerable overlapping of bands characteristic of primary, secondary, and tertiary alcohols. Thus we should expect to find bands characteristic of the C–O stretching of the C–O–H group in the spectra of glycerides at longer wavelengths. Table IV shows that bands are observed at 9.5 and 9.6 microns in the spectra of all glycerides which contain the C–O–H group.

The band with maximum at 9.6 microns is observed only in the spectra of diglycerides (with the single exception of dipalmitolactin, the spectra of which resembles that of a diglyceride). It would appear logical therefore to assign this band to the C–O stretching of an alpha substituted secondary alcohol, a correlation not incompatible with the conclusions of Zeiss and Tsutsui (26). The band arising from C–O stretching of alpha substituted primary alcohols (at 9.6 microns in the spectra of straight-chain unsubstituted compounds) would be shifted above the 9-micron region considered here. It is significant perhaps to observe that the spectra of all monoglycerides which contain a primary alcohol exhibit bands with maxima between 10.1 and 10.2 microns, not observed in the spectra of di- and triglycerides. In the spectra of the monoglycerides the shift in frequency of the C–O stretching band of the secondary alcohol might be expected to be somewhat different from that exhibited by the diglycerides. In the spectra of all monoglycerides a band is exhibited with maxima at 9.5 microns, and an inflection is noted at 9.4 microns. The band at 9.5 microns could be correlated with a C–O stretching of an alpha substituted secondary alcohol in a monoglyceride as distinguished from the similar stretching in a diglyceride at 9.6 microns.

Whether these suggested correlations are entirely correct, a significant fact from the standpoint of use of the spectra for analytical purposes evolves. Monoglycerides can be detected by observation of a band with maximum at 9.5 microns and determined by consideration of the intensity of this band. Diglycerides can be detected and determined by use of the 9.6-micron band. Triglycerides can then be obtained by difference. Absence of any bands between 9.1 and 10.0 microns can be construed as evidence for a pure triglyceride.

In the spectra of the mixed short- and long-chain glycerides (Table IV) both triacetin and tributyrin exhibit weak broad bands in the region of 9.5 microns which would interfere with the determination of monoglyceride content in admixtures containing triacetin or tributyrin and monoglycerides. This band is not observed in the spectra of most of the diaceto- and dibutyro-compounds. Its appearance in the spectra of the palmitins would appear to be an indication of monoglyceride impurity. This fact is in need of further verification. The inflection at 9.4 microns, observed in the spectra of most of these compounds, would not interfere with the determination of monoglyceride content at 9.5 microns, and there are no bands observed in these spectra which would interfere with the determination of diglyceride content at 9.6 microns.

TABLE V

Absorption Bands in the Region of C–H Bending About a Trans C=C Group, 10μ

Glyceride	Intensity at maxima	
	10.3μ	10.4μ
Tristearin	.....	.....
Tripalmitin	.....	.....
Triolein	0.119	.....
Trielaidin	0.358	.....
1,3-Distearin	.....	.....
1,3-Dipalmitin	.....	.....
1,3-Diolein	.....	.....
1-Aceto-3-stearin	.....	.....
1-Monostearin	.....	.....
1-Monopalmitin	.....	.....
1-Monoolein	.....	.....
1-Monomyristin	.....	.....
1,3-Dipalmito-2-lactin	.....	.....
Triacetin	.....	0.368
1,2-Diacetostearin	.....	0.178
1,2-Diacetopalmitin	.....	0.196
1,2-Diacetoolein	.....	0.176
Tributyrin	.....	0.254
1,2-Dibutyrostearin	.....	0.154
1,2-Dibutyropalmitin	.....	0.162
1,2-Dibutyroolein	.....	0.152

Interference from the spectra of triacetin or tributyrin could be eliminated by suitable correction factors. An important principle in applying infrared spectra to quantitative methods can be illustrated here. If the problem is to determine the percentage of mono- or distearin in a sample of tristearin, absorptivities obtained from pure samples of the mono- and distearins should be employed with correction factors for background, if required, based on the spectra of pure tristearin. This procedure might be somewhat broadened to include determinations for any mono- and di- long-chain glycerides in the presence of any long-chain triglyceride by the use of average values. However, if the problem involves the determination of monostearin in 1,2-aceto-3-stearin prepared from it, absorptivities obtained from pure monostearin and "background" correction factors based on the spectra of the diaceto-compound and probably on triacetin, if its presence is suspected, should be employed. Another application of this principle will be mentioned in connection with the discussion of the use of the C–H bending vibrations in the 10-micron region to determine the total trans-isomers.

As observed in the 3.0-micron region, the spectra of the triglyceride, dipalmitolactin, resembles that of a diglyceride with a band at 9.6 microns. This band most probably arises from a C–O stretching of the secondary alcohol in the lactic acid portion of this molecule. Its spectrum again demonstrates that the analytical procedure suggested here cannot be employed for the analysis of materials containing hydroxyglycerides.

The 10.0 micron—C–H bending vibration about the trans C=C group. An absorption band with maximum at 10.3 microns, which has been shown to arise from a C–H bending about a trans C=C (15), has been used to determine quantitatively trans-isomers

in monounsaturated fatty acids, esters, and glycerides (11, 16, 19). If the assumption is made that the intensity of the C–H bending about the trans C=C group is additive in nonconjugated polyunsaturated compounds (1, 12), the method can be extended to the determination of total trans-isomers, expressed as elaidic acid, in these compounds (5).

In Table V this C–H bending about the C=C trans group is observed as a sharp band at 10.3 microns in the spectrum of trielaidin, the only pure trans-compound included in this study. A weak band can be observed in the spectrum of triolein, showing that this cis-compound contains a trace of trans-impurity.

Although the quantitative method of Shreve, Heether, Knight, and Swern (16), extended by the assumption that the C–H bending is additive in nonconjugated compounds, is reasonably satisfactory for the analysis of normal long-chain glycerides, its use to determine total trans-isomer content of the mixed short- and long-chain glycerides results in anomalously high values. Table V shows the reasons for the high results. These compounds exhibit a band with maxima at 10.4 microns. The "shoulder" of this band interferes with measurements at about 10.3 microns. It can be shown that the intensity of this band increases as the chain length of the fatty acids in the glycerides decrease.

Again, application of the principle that quantitative procedures based on infrared absorption measurements must consider the total composition of the sample being analyzed should result in a satisfactory determination. If the problem is the determination of trielaidin in the presence of triolein and tristearin, absorptivities based on very pure trielaidin and correction factors for "background" based on the absorptions of triolein and tristearin at the maxima found for trielaidin are required, as used in the method of Shreve *et al.* (16). If however the content of 1,2-diacetoelaidin in the presence of 1,2-diacetoolein and triacetin is required, coefficients based on the spectrum of very pure 1,2-diacetoelaidin and "background" correction factors based on the observed spectra of very pure 1,2-diacetoolein and triacetin are required for a satisfactory analysis.

This principle requires that extension of methods for quantitative analysis based on infrared absorption measurements must be accompanied by careful measurement and evaluation, under the exact conditions by which subsequent analyses will be made, of coefficients of the very highly purified compounds. Thus extension of the present method for the quantitative determination of trans-isomers in monounsaturated compounds to polyunsaturated materials must await a careful quantitative evaluation of the infrared spectra of the polyunsaturated compounds. Similarly, extension of a method to determine trans-isomers in long-chain glycerides to mixed short- and long-chain glycerides must await similar evaluation of very highly purified mixed glycerides. Until compounds to permit these quantitative evaluations are made available, infrared methods, at best, can only be semi-quantitative.

Summary

The infrared spectra from 2 to 12 microns of chloroform solutions of several glycerides have been measured and studied with a view to possible analytical applications. These spectra are presented, and conclusions which can be obtained from their examination are reported in this paper.

The principal bands, common to the spectra of all glycerides, have been tabulated with correlations of the vibrating groups which give rise to them. The analytical significance of the infrared spectra is considered in detail for three specific regions: a) the O–H stretching vibration region, about 3.0 microns; b) the C–O stretching vibration region, about 9.0 microns; and c) the 10.0-micron region of C–H bending, about the C=C group.

Analyses of these regions of the spectra indicate that infrared absorption can be used to detect and to determine mono-, di-, and triglycerides in admixtures and that the method for the determination of trans-isomers can, with modifications, be extended to include analysis of triglycerides.

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