Relationship Between the Calculated Glyceride Composition and the Iodine Value of Cottonseed and Pecan Oils

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Abstract

The concentrations of the major component glyceride types in cottonseed and pecan oils were calculated at selected iodine values from the fatty acid compositions of the oils using the Gunstone equations. The relative concentrations of the glycerides change markedly with increasing iodine value. In cottonseed oil the concentrations of the PLL and LLL glyceride types, for example, increase from 19.5 to 26.3% and from 6.5 to 16.7%, respectively, for an iodine value change from 95 to 112. In pecan oil the concentration of the OOL glycerides goes through a maximum at an iodine value of 110. The concentrations of the OLL and OOO glycerides show a tenfold increase and fivefold decrease, respectively, as the iodine value increases from 90 to 120.

Graphs are presented which permit the estimation of the glyceride composition of random cottonseed or pecan oils of know iodine value. These will be useful in the selection of these oils as source materials in the production of tailor-made fats and oils or other edible or inedible industrial products.

Introduction

THE DETERMINATION of the glyceride composition of oils has long been the subject of investigation. Various methods of analysis have been employed and several theories have been developed which form the basis for calculating the proportions of the various types of glycerides in an oil from its fatty acid composition (1).

Numerous reports have been published comparing the calculated glyceride compositions of specific samples of vegetable oils with the experimental data (1). To date, however, no attempt has been made to show how the glyceride composition of a given oil changes with the iodine value of the oil.

Only recently, by the application of GLC analysis, have reliable data on the fatty acid composition of oils become available. A recent publication from this Laboratory (2) reports the fatty acid compositions of a series of cottonseed oils having a wide range of iodine values and representing a large number of commercial varieties of cottonseed. In an earlier publication French (3) reported the fatty acid compositions of a similar series of pecan oils. From these data it is possible to calculate the glyceride composition of these two oils at a number of different iodine value levels and thus, determine to what extent the glyceride composition of an oil is affected by changes in iodine value. The Gunstone equations (4, Theory I) were used in these calculations since for vegetable oils they have been shown to give results which closely approximate those obtained by experimental analysis (5–7).

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Procedure and Results

The fatty acids of pecan oil consist mainly of oleic, linoleic, stearic, and palmitic acids. The concentrations of stearic acid, about 6.5%, and palmitic acid, about 2.5%, are relatively independent of the iodine value. On the other hand, the oleic acid content decreases linearly from 76% to 51% and the linoleic acid content increases linearly from 14% to 28% as the iodine value varies from 94 to 118. It is interesting to note, however, that the average combined concentration of oleic and linoleic acids is remarkably constant, about 89.6%, over the entire range of iodine values, with a maximum of 90.6% and a minimum of 88.8%.

The changes in the concentration of oleic and linoleic acids with the iodine value are represented by the following regression equations:

$$\%\ \text{oleic acid} = -1.0708\ (\text{I.V.}) + 176.86 \qquad [1]$$

$$\%\ \text{linoleic acid} = +0.9917\ (\text{I.V.}) - 79.42 \qquad [2]$$

The standard deviations calculated from these equations, $\pm 0.7\%$ for oleic acid and $\pm 0.7\%$ for linoleic acid, illustrate the high degree of correlation between the concentration of these acids and the iodine value of the oil. Similar equations for the change in the concentration of the major fatty acids with iodine value have already been reported for cottonseed oil (2).

Fatty acid compositions at selected iodine values

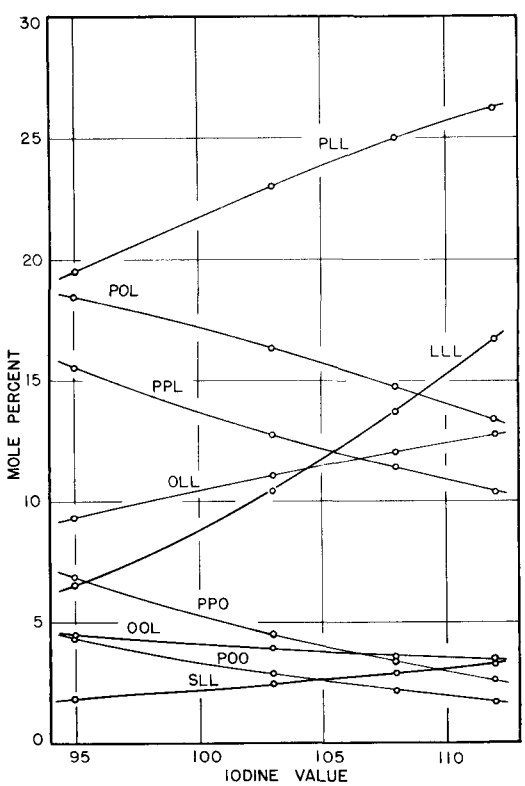

FIG. 1. Calculated glyceride compositions vs. iodine value for cottonseed oil.

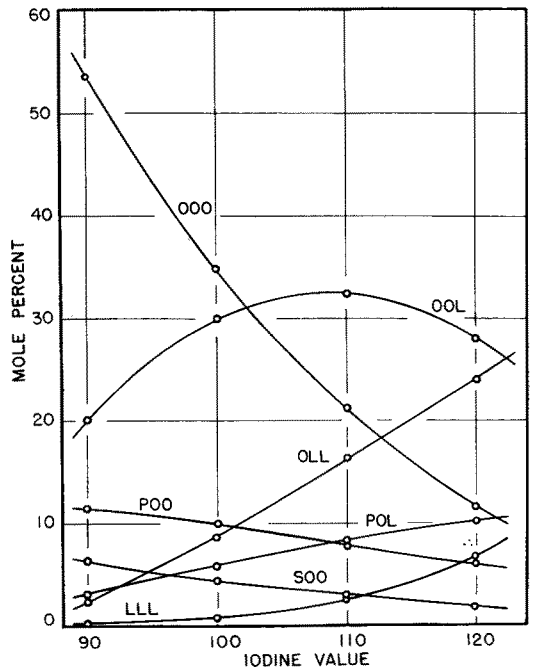

FIG. 2. Calculated glyceride compositions vs. iodine value for pecan oil.

were obtained from the regression equations for both cottonseed and pecan oils. The concentration of the component glycerides were then calculated at these iodine values by substitution of the molar percentage of the acids in the Gunstone equations. The relationship between the concentration of the major glyceride types and the iodine value of the oils is illustrated in Fig. 1 and 2. The symbols PSL, POO, etc., denote only the acids present and not the position of the acyl groups. P stands for palmitic; S, stearic; O, oleic; and L, linoleic.

The results show that the glyceride composition of the oil as well as the concentration of the various glyceride types are markedly affected by changes in the iodine value.

In the case of cottonseed oil it will be noted from Fig. 1 that oils of high iodine value are much richer in glycerides of the structure PLL, LLL, and OLL, and have much lower concentrations of POL, PPL, PPO and POO. The concentrations of PLL and LLL increase from 19.5 to 26.3%, and from 6.5 to 16.7%, respectively, as iodine value changes from 95 to 112, while the concentrations of POL, PPL, and PPO decrease from 18.4 to 13.4%, 15.5 to 10.4%, and 6.9 to 2.6%, respectively. With the exception of SLL, which shows a slight increase, and OOL, which shows a slight decrease with increasing iodine value, the remaining glycerides show no marked change.

The change of glyceride composition with iodine

TABLE I

Experimental and Calculated Glyceride Composition of a Cottonseed Oil (I.V. 112)

Glyceride type	Mole % glyceride		Glyceride type	Mole % glyceride	
	Calculated	Literature[a]		Calculated	Literature[a]
PPO	2.6	4.1	PPL	26.3	26.6
SSO	0.0	.....	SLL	3.2	1.7
PPL	10.4	9.6	POL	13.4	15.9
SSL	0.2	0.0	SOL	1.6	1.1
PSO	0.7	1.0	OOO	0.3	0.4
PSL	2.5	1.5	LLL	16.7	16.9
POO	1.7	2.5	OLL	12.7	14.2
SOO	0.2	.....	OOL	3.2	3.1

[a] Reference 5.

value in pecan oil is particularly interesting (see Fig 2). At an iodine value of 90 the concentration of the OOL glycerides is about 20%. It increases to a maximum of about 32% at an iodine value of about 110 and then decreases to about 29% as the iodine value increases to 120. The concentration of the OLL glycerides undergoes a 10-fold increase (2.5 to 23.9%) over the same iodine value range while that of the OOO glycerides shows a fivefold decrease (53.6 to 11.6%). The concentration of LLL, only about 0.1% at the lower iodine values, increases very slowly at first and then more rapidly to about 6.6% at an iodine value of 120. The POL, POO, and SOO glycerides are less affected by iodine value changes; POL increases from 2.8 to 10.1% and POO and SOO decrease from 11.4 to 6.1% and 6.3 to 1.8%, respectively.

The results show that the glyceride composition of an oil is highly dependent upon the iodine value of the oil and may be expected to be quite different for random samples of a given oil. That the calculated glyceride compositions are realistic is indicated by the comparative data for cottonseed oil in Table I. The calculated data for the oil of iodine value 112.0 is in close agreement with that determined experimentally by Vereshchagin et al. (5) for cottonseed oil of iodine value 111.9. It follows that if the iodine value of a given cottonseed or pecan oil is known, a reasonable estimate of its glyceride composition can be made from Fig. 1 or 2.

It is apparent that a knowledge of the relationship between the glyceride composition and iodine value of an oil is of fundamental importance in the selection of source material for tailor-made fats and oils, or other edible or inedible industrial products.

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