High Resolution ^{13}C N.M.R. Spectra of the Carbonyl Carbons of the Triglycerides of Palm Oil

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The qualitative composition of palm oil triglycerides can be obtained by ^{13}C n.m.r. analysis of the oil.

Palm oil is composed mainly of triglycerides of the fatty acids palmitic, oleic, linoleic, and stearic acid.[1] The oil that is derived from the oil palm fruits exists at ambient temperatures (25—35 °C) in two phases, a liquid (palm olein) and a solid (palm stearin). It is known that the melting point of palm oil generally depends on the composition of the triglycerides; the larger the proportion of unsaturated fatty acids the lower is the melting point.

The high resolution ^{13}C n.m.r. spectrum of the carbonyl carbons of the triglycerides, Figure 1, shows that the carbonyl carbons of saturated, oleic, and linoleic acids can be distinguished. The carbonyl carbons of saturated chains attached to either of the 1,3-glyceridic carbons appear at the same position as the highest frequency peak in the spectrum [at δ 173.05 $\pm$ 0.01 in dilute solution in $CDCl_3$ (conc. 1 : 3 v/v)] while those of oleic and linoleic acids attached to the same glyceridic carbons appear at slightly lower frequencies (that of oleic acid differs by 0.029 $\pm$ 0.002 p.p.m. while that of linoleic acid differs by an additional 0.012 $\pm$ 0.002 p.p.m.). In Figure 1, the linoleic peak appears as a shoulder on the low frequency side of the oleic peak. The carbonyl carbons of saturated fatty acids attached to the 2-glyceridic carbon

appear at δ 172.68 ± 0.01 while those of oleic and linoleic acids appear at slightly lower frequencies, differing by the same amounts as those attached to the 1,3-glyceridic carbons. This assignment of the carbonyl carbon peaks was verified by examining the same spectra of mixtures of synthetic triolein and tripalmitin as well as the spectra of corn oil and its mixtures with the former two.

Figure 1 also shows the spectra of the carbonyl carbons of various fractions of palm oil, corn oil, and cocoa butter. Comparing spectrum (b) for palm stearin (m.p. 46—58 °C) and spectrum (d) for palm olein, which is a liquid at room temperature (22 °C), it can be deduced that, while the ratio of saturated to unsaturated chains attached to the 1,3-glyceridic carbons is not appreciably different in these two fractions of palm oil, the proportion of triglycerides having saturated fatty acids attached to the 2-glyceridic carbon is significantly larger in the case of palm stearin (or the proportion having oleic and linoleic acids is significantly larger in the case of palm olein). As expected, the spectrum (a) of palm oil shows the proportion of saturated and unsaturated acids as being intermediate between those of its two fractions. Spectrum (c) is that of a higher melting ('hard') fraction of palm stearin (m.p. 52—54 °C) and shows that a greater proportion (>60%) of the triglycerides have saturated fatty acids attached to the 2-glyceridic carbon and that most (*ca.* 90%) of the fatty acids attached to the 1,3-glyceridic carbons are saturated. The spectrum (f) of cocoa butter (m.p. 30—35 °C) is similar to that of 'hard' palm stearin in that nearly all of the 1,3-glyceridic carbons have saturated acids attached to them; they differ in that all the cocoa butter triglycerides have oleic and, to a smaller extent, linoleic acids at the 2-glyceridic carbon. Spectrum (e) for corn oil shows that the major fatty acid component is linoleic, that essentially all the saturated fatty acids are attached to the 1,3-glyceridic carbons, and that essentially all the fatty acids attached to the 2-glyceridic carbon are unsaturated, mainly, linoleic.

This ability to infer the nature of the fatty acid chain attached to the glyceridic carbons by ^{13}C n.m.r. analysis is of significance to the palm oil industry as palm oil has a relatively high composition (*ca.* 20%) of triglycerides having saturated fatty acids attached to the 2-glyceridic carbon.

The proton-decoupled ^{13}C spectra were recorded on a JEOL JMN FX100 Fourier-transform n.m.r. spectrometer operating at 25.05 MHz with the following parameters: data memory 8 k, spectral width 200 Hz, acquisition time 10.24 s, pulse delay 0.5 s, and pulse angle 45°. From the integrated intensities the two sets of peaks were consistently found to exhibit the theoretical 2:1 ratio and hence the same nuclear Overhauser enhancement.

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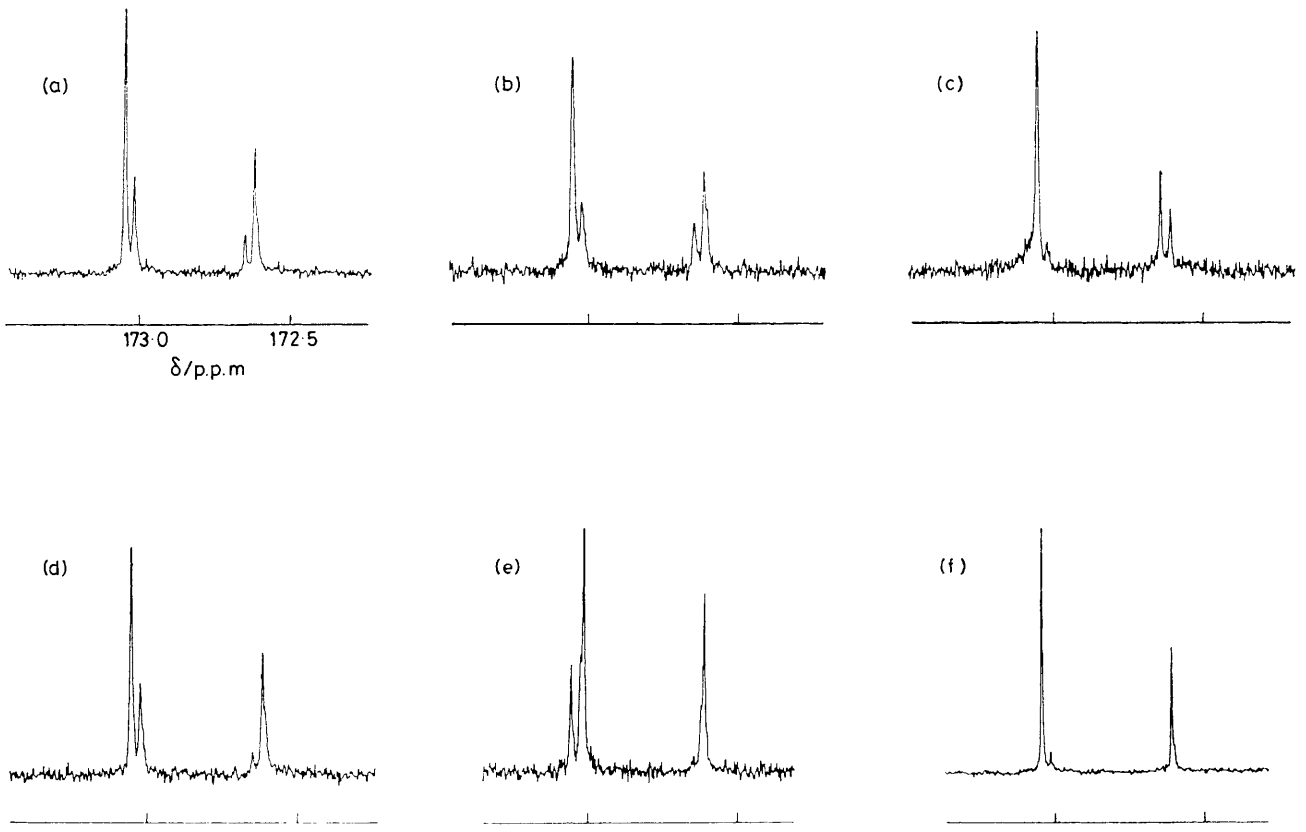

Figure 1. Proton-decoupled high resolution ^{13}C n.m.r. (25.05 MHz, 28 °C) of the carbonyl carbons of the triglycerides in (a) palm oil, (b) palm stearin (m.p. 46—58 °C), (c) 'hard' palm stearin (m.p. 52—54 °C), (d) palm olein, (e) corn oil, and (f) cocoa butter. Samples (a), (b), (c), and (f) were homogenised before use.