is necessary to apply empirical corrections. If this is properly carried out it is possible to determine the percentage of the various components of the mixture directly. If pure components are available it is easy to check the results by running artificial mixtures and thus to get a very high accuracy in the quantitative analysis.

The mass spectra of the samples of methyl linoleate and methyl linolenate studied show a peak at $m/e = 290$. In the case of methyl linoleate the height of this peak is 1.7 % of the parent peak ($m/e = 294$). For methyl linolenate the height of the $m/e = 290$ peak is 18 % of the parent peak at $m/e = 292$. This peak appears to be the parent peak of the methyl ester of a C_{18} acid containing four double bonds. Whether this acid is present as an impurity in the original samples or whether it is formed by a dehydration reaction in the heated intake system of the mass spectrometer cannot be said at present. The present evidence, however, is in favour of the first mentioned possibility. It has been proposed that acids of this type may be formed from linoleic and linolenic acids by dehydrogenation between the existing double bonds and the carboxyl group in such a way that all unsaturation is methylene-interrupted and all *cis*. (*cf.* Ref.[5]). C_{18} tetra-ethenoid acids have been found in the fats of marine animals [5, 6].

In a complex mixture it is not possible to distinguish between geometrical and positional isomers within each group of unsaturated esters. The peak at $m/e = 296$ in the figure might thus be due to, *e.g.*, methyl oleate (methyl *cis*-$\Delta^{9:10}$-octadecenoate), methyl elaidate (methyl *trans*-$\Delta^{9:10}$-octadecenoate), or methyl petroselinate (methyl *cis*-$\Delta^{6:7}$-octadecenoate) or due to a mixture of mono-ethenoid esters. It may be possible to overcome this difficulty by examining suitable derivatives.

The high-mass, high-resolution mass spectrometer thus offers a convenient method for determining the fatty acid distribution ("fatty acid spectrum") of natural or synthetic fats. The analysis can be performed on a few milligrams of material.

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Note on the Crystal Structure of Niobium Monoxide

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In connection with studies on transition metal compounds of defective sodium chloride structure, *e.g.* vanadium monoxide [1] and titanium monoxide [2], the powder pattern of niobium monoxide was registered by means of an X-ray G.M. diffractometer (Cu*K* radiation). The structure derived by Brauer [3] for this substance (a defective sodium chloride structure with the positions 000 and ½½½ vacant) is supported by our measurements, but as our investigation is based on quantitative data it may be worth mentioning.

The lattice parameter of the niobium monoxide sample as obtained from a Guinier powder photograph (internal standard potassium chloride $a = 6.2919$ Å at 20°C) was found to be 4.210_8 Å in excellent agreement with the value given by Brauer 4.2103 ± 0.0004 Å (21°C). The density was found to be 7.3 likewise in perfect agreement with Brauer's value of 7.30 and the value 7.27 calculated for a cell content of three formula units of NbO.

Table 1 gives the *F* values for the first fourteen reflexions as obtained from the diffractogram. The alternative structures (2)—(4) are among those discussed by Brauer *viz.* 3 Nb in ½½0, ½0½, 0½½ for (2)

Table 1. X-Ray diffractometer data for niobium monoxide.

hkl	F_{obs}	F_{obs}—F(Nb)	Structure (2)		Structure (3)		Structure (4)	
			F_{calc}	F(O)	F_{calc}	F(O)	F_{calc}	F(O)
100	$\overline{32}$	4	$\overline{29}$	8	$\overline{36}$	0	$\overline{25}$	11
110	$\overline{38}$	$\overline{4}$	$\overline{40}$	$\overline{6}$	$\overline{34}$	0	$\overline{34}$	0
111	73	$\overline{21}$	78	$\overline{16}$	78	$\overline{16}$	86	$\overline{8}$
200	100	11	104	14	104	14	104	14
210	$\overline{25}$	3	$\overline{24}$	4	$\overline{28}$	0	$\overline{22}$	6
211	$\overline{34}$	$\overline{7}$	$\overline{31}$	$\overline{4}$	$\overline{27}$	0	$\overline{27}$	0
220	79	4	85	10	85	10	85	10
221	$\overline{22}$	2	$\overline{21}$	3	$\overline{24}$	0	$\overline{20}$	5
300	$\overline{22}$	2	$\overline{21}$	3	$\overline{24}$	0	$\overline{20}$	5
310	$\overline{26}$	$\overline{2}$	$\overline{27}$	$\overline{3}$	$\overline{24}$	0	$\overline{24}$	0
311	58	$\overline{11}$	61	$\overline{8}$	61	$\overline{8}$	65	$\overline{4}$
222	80	13	75	8	75	8	75	8
320	$\overline{22}$	0	$\overline{20}$	2	$\overline{22}$	0	$\overline{18}$	4
321	$\overline{24}$	$\overline{3}$	$\overline{24}$	$\overline{2}$	$\overline{21}$	0	$\overline{21}$	0

—(4) and 3 O in $\frac{1}{2}00$, $0\frac{1}{2}0$, $00\frac{1}{2}$ (structure (2)), 3 O randomly distributed in $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}00$, $0\frac{1}{2}0$, $00\frac{1}{2}$ (structure (3)) and 3 O randomly arranged in 000, $\frac{1}{2}00$, $0\frac{1}{2}0$, $00\frac{1}{2}$ (structure (4)). For each of the structure alternatives, the values of F_{calc} for the two components of the unresolved reflexion (221 + 300) are identical and the corresponding values of F_{obs} are thus calculated considering the multiplicity of the reflexions. The signs alloted to F_{obs} are those determined by the arrangement of the Nb atoms.

The consistency is definitely better for structures (2) and (3) than for (4) (and for still another structure (5) discussed by Brauer). The difference between F_{calc} and F_{obs} for (2) and (3) is relatively small, as may be anticipated from the similarity of these two alternatives, but the data speak in favour of structure (2) in accordance with Brauer's opinion. The quotients $\Sigma||F_{\text{obs}}| - |F_{\text{calc}}||/\Sigma|F_{\text{obs}}|$ are 0.058, 0.079 and 0.109 for (2), (3) and (4), respectively. The table also gives the differences between F_{obs} and F(Nb) (the contribution of the niobium atoms to F_{calc}) which may represent the share in F_{obs} of the oxygen atoms. The quotients $\Sigma||F_{\text{obs}} - F(\text{Nb})| - |F(\text{O})||/\Sigma|F_{\text{obs}} - F(\text{Nb})|$ are 0.44 for (2), 0.56 for (3) and 0.78 for (4).

Melting of niobium monoxide (small tablets) in an electric arc furnace with subsequent rapid quenching from the melting temperature did not change the structure of this compound. Evidently there is no indication of a phase transition similar to that found in titanium monoxide [2]. Thus high-temperature studies would be necessary to decide definitely whether there occurs a rapid transition to a random niobium monoxide at a certain temperature.

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