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Letter to the Editor

Computer processing of fatty acid analysis data

Sir,

Recently, Aston[1] presented a Fortran program for processing fatty acid data which computes the concentrations of each fatty acid, the percentage of glycerol, the theoretical iodine value, etc. It allows processing of a large amount of data and may be of value to those who are not familiar with computer programming. However, we noticed that the program does not take into account the amount of water lost during esterification of the fatty acids with glycerol, and thus the amount of fat formed from 100 g of fatty acids is overestimated. This gives rise to an appreciable underestimation of the "theoretical iodine value" and weight % of glycerol.

Since 1 mole of fat is formed by the esterification of 1 mole of glycerol with 3 moles of fatty acids and the elimination of 3 moles of water, the amount of fat (WF) from 100 g of fatty acids (f.a.) may be calculated as:

$$WF = 100 + \sum_{1}^{n}\left(\frac{\text{Wt. \% of f.a.}}{\text{Mol. wt. of f.a.}}\right)_i \left(\frac{92.09}{3} - 18.02\right) \text{ or}$$

$$WF = 100 + (\text{moles of glycerol associated with 100 g of f.a.}) \times \times (92.09 - 18.02 \times 3) \quad (1)$$

The addition of iodine to 100 g of fatty acids is correctly represented by ii (ref. 1, p. 123, line 42) if the term "iodine equivalent" (= the number of gram atoms of iodine bound to 100 g of fatty acids) replaces "iodine mole equivalent". The iodine value (IV_T) may then be estimated from gas chromatographic analysis (ref. 1, p. 123, iv, line 48) as:

$$IV_T = \text{"theoretical iodine value"} = \frac{\text{Weight of iodine associated with 100 g of f.a.'s}}{WF} \times 100 \quad (2)$$

Accordingly, the wt.% of glycerol in fat should be given by (*cf.* ref. 1, p. 123, vi, line 30):

$$\frac{\text{Weight of glycerol residues associated with 100 g of f.a.'s}}{WF} \times 100 \quad (3)$$

Neglect of the amount of water eliminated during esterification gives rise to an underestimation of the "theoretical iodine value" of 5–7% depending on the mean molecular weight of the fatty acids $\overline{(\text{Mol. wt.})}$ in the fat. The deviation (ΔIV_T) between the true "theoretical iodine value" and that presented by Aston[1] may be estimated from the expression:

$$\text{Error \%} = \frac{\Delta IV_T}{IV_T} \times 100 = 100\left(1 - \frac{\overline{(\text{Mol. wt.})} + 12.683}{\overline{(\text{Mol. wt.})} + 30.699}\right) \quad (4)$$

Taking butter fat ($\overline{\text{Mol. wt.}} = 230$) and horse fat ($\overline{\text{Mol. wt.}} = 280$) as typical examples, errors of 6.9 and 5.8% respectively are calculated.

The program may be corrected according to eqns. 3 and 2 by changing statement numbers 76 and 77 (ref. 1, p. 128, lines 6 and 10):

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C   GLCW = WEIGHT OF FAT DERIVED FROM 100 GM OF FATTY
    ACIDS
(75) GLMT = GLCM + GLMN
(76) GLCW = GLMT * 38.049
C
C   COGL = PERCENT GLYCEROL RESIDUES IN FAT
(77) COGL = GLMT * 89.071 * 100/(100 + GLCW)
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As part of graduate training in fat analysis[2], students of the faculty have to check "theoretical iodine values", calculated from gas chromatograms, against the values obtained by direct titrimetry of the fat[3]. We have found that for dry fats there is generally close agreement between the experimental and calculated iodine values. However, significantly lower "theoretical iodine values" than titrimetric values are calculated if higher unsaturated fatty acids are missing from the chromatogram.

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1 J. W. Aston, *J. Chromatogr.*, 131 (1977) 121.
2 R. Verbeke, *Scheikundige analyse der eetwaren van dierlijke oorsprong*, Graduate course, Veterinary Faculty, Univ. Ghent, 1973.
3 H. Pardun, *Handbuch der Lebensmittelchemie, Bd. IV, Lipids*, Springer, Berlin, 1969, p. 573.

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Reply

Sir,

The alteration to the equation for the calculation of the theoretical iodine value in the above paper by Drs. De Brabander and Verbeke is correct. The failure to account for the loss of water of esterification was an oversight on my part. I will enclose correction notes with all future reprint requests.

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