SUGAR CALCULATIONS.

By J. F. LIVERSEEGE, F.I.C.

A PUBLIC ANALYST in the examination of substances containing sugars has to use constants and equations. The following notes are the results of an attempt, by selection and calculation, to obtain a set of data that is clear and consistent.

SPECIFIC ROTATORY POWER.—There are ambiguities in published specific rotatory powers owing to authors failing to state the temperature and concentration of the solutions used, and sometimes it is not clear whether the sugar was anhydrous or contained water of crystallisation. In some cases results given by various authorities differ considerably, and the selection of the best value has been difficult. This particularly applies to *lævulose* and invert sugar. The value for invert sugar should be half the algebraic sum of those of *lævulose* and *dextrose*. The selected values for sugars are given in the table on p. 450. In practice it is a convenience to apply the term "specific rotatory power" not only to pure sugars, but also to mixed substances such as treacle.

CORRECTION FOR TEMPERATURE.—In factors given for the correction of specific rotatory power there often is doubt as to whether in the equations given the sign for left-handed rotation (–) is to be used as well as any algebraical sign. As the temperature correction will never alter the rotation from "+" to "–," it is better to ignore the optical signs in making this correction.

Equation (1), given below, is to be used when the specific rotatory power of a pure sugar is being determined; equation (2) when the actual angle of determination is being corrected for temperature. In this case, α^{20} means the angle at 20° C. of a solution examined in a 200 mm. tube; $[\alpha]_D$ may be substituted for α in this equation. The values for "D" and "d" are given in the table, and "t" represents degrees C.

$$(1) [\alpha]_D^{20} = [\alpha]_D^t + D(t - 20). \quad (2) \alpha^{20} = \frac{\alpha^t}{1.0 + d(20 - t)}.$$

The application of equation (2) may be illustrated by the correction for temperature of a solution of invert sugar, which gave a rotation of -7.7° at 24.4° C.:

$$\alpha^{20} = \frac{7.7}{1.0 + 0.0149(20 - 24.4)} = 8.24^\circ.$$

Solutions should be made up to volume at 20° C., and polarised as near this standard temperature as is convenient.

CORRECTION FOR CONCENTRATION.—The standard concentration is 10 *w/v* (*i.e.*, 10 grms. per 100 c.c.). When a sugar solution is diluted, in addition to the primary reduction of the angle according to the equation,

$$(3) \alpha = \frac{w/v \times [\alpha]_D}{50},$$

there is with some sugars a secondary reduction, owing to the fact that in dilute solutions the rotatory power *per unit of sugar* is less than in stronger solutions.

The sign $[\alpha]_D^{20}$ is often used to indicate the specific rotatory power of a sugar at

20° C. when a sodium flame is used. A useful extension of it is to add the figure for the w/v of the solution to the left-hand side of the bracket. The sign $^{10}[\alpha]^{20}$ would therefore mean that the specific rotatory power was corrected to 20° C., and that the figure was also corrected for this secondary alteration to 10 w/v . The corresponding sign for the angle actually observed in a 200 mm. tube is $^{10}\alpha^{20}$. Again, to avoid ambiguities, the optical signs of the sugar solutions are ignored in making the correction.

Equation (4) is to be used for correcting the specific rotatory power of sugar to the standard of 10 w/v when the concentration is known. In many cases, however, the concentration of the solution has to be determined, and therefore cannot be used. In such cases an approximation may be made by using the determined angle in place of the w/v , as in equation (5). The values for " C ," " c ," and " B ," are taken from the table :

$$(4) \quad ^{10}[\alpha]_D = [\alpha]_D + C (10 - w/v).$$

$$(5) \quad ^{10}\alpha^{20} = \alpha^{20} + c (B - \alpha^{20}) \alpha^{20}.$$

The above-mentioned solution of invert sugar may be taken as an example of equation (5) :

$$^{10}\alpha = 8.24 + 0.0080 (4.2 - 8.24) 8.24 = 7.98^\circ.$$

CALCULATION OF w/v WHEN ONE SUGAR ONLY IS PRESENT.—Either of the following equations may be used :

$$(6) \quad \text{Sugar } w/v \text{ in the solution} = \frac{50 \times ^{10}\alpha^{20}}{^{10}[\alpha]_D^{20} \text{ of pure sugar}}.$$

$$(7) \quad \text{Sugar } w/v \text{ in the solution} = \frac{10 \times ^{10}\alpha^{20}}{B}.$$

Applying this to the above-mentioned solution of invert sugar,

$$\frac{50 \times 7.98}{21} \text{ or } \frac{10 \times 7.98}{4.2} = 19.0 \text{ } w/v;$$

and as 100 c.c. contained 19.2 grms. of the substance, the percentage of invert sugar present = $\frac{19.0 \times 100}{19.2} = 99$ per cent.

With specific rotatory powers the following equation may be used :

$$(8) \quad \text{Sugar per cent. (by weight) in the substance} = \frac{100 (^{10}[\alpha]_D^{20} \text{ of substance})}{^{10}[\alpha]_D^{20} \text{ of pure sugar}}.$$

MIXTURE OF TWO SUGARS.—Solutions of sucrose which is partly inverted often require examination. On inversion, 100 parts of sucrose yield 105 parts of invert sugar. In many cases it is more convenient to express invert sugar in terms of the sucrose from which it was derived, and I have used the term "inverted sucrose" to indicate this result. Unless it is known that only two sugars are present, it is necessary to prove by the determination of the reduction and total organic solids that such is the case. A mixture of sucrose and invert sugar in suitable proportions is optically inactive.

SUCROSE AND INVERTED SUCROSE.—When the substance consists of sucrose which has been partly inverted, the following equations will give its composition. " I " is used for the angle after inversion, corrected for temperature and concentra-

tion by equations (2) and (5), and α for the original angle of polarisation at the same dilution as " I ":

- (9) Sucrose w/v in solution = 0.565 (change of angle of rotation).
- (10) Inverted sucrose w/v originally present = 0.565 ($3.023 I \pm \alpha$).
- (11) Angle due to sucrose = 0.75 (change of angle of rotation).
- (12) Angle due to inverted sucrose originally present = 0.249 ($3.023 I \pm \alpha$).

In equations (9) and (11) the change of rotation will be the sum of the angles if the sign of rotation is altered by inversion, and their difference if their signs are the same.

In equations (10) and (12) " $-$ " is used if the sign of the optical rotation is changed by inversion. If these equations give a negative result, dextrose, and not inverted sucrose, is present.

SUCROSE AND DEXTROSE.—The corresponding equations for mixtures of sucrose and dextrose are:

- (13) Dextrose w/v = 0.235 ($\alpha \pm 3.023 I$).
- (14) Angle due to dextrose = 0.249 ($\alpha \pm 3.023 I$).

The " $-$ " sign is used if inversion changes the optical sign.

DEXTROSE AND LÆVULOSE: INVERT SUGAR.—If dextrose and lævulose are present in equal quantities they become invert sugar. If the quantities are dissimilar, a mixture of invert sugar with excess of lævulose or dextrose results, and the composition can be calculated in either form by the following equations:

- (15) Per cent. of invert sugar = $1.35 (52.8 - {}^{10}[\alpha]^{20})$.
- (16) Per cent. of lævulose = $0.678 (52.8 - {}^{10}[\alpha]^{20})$.

In these equations the optical signs must be included as well as the algebraic ones.

CORRECTION FOR TEMPERATURE AND CONCENTRATION OF A MIXTURE OF TWO SUGARS.—As sucrose and inverted sucrose polarise in opposite directions, the angle of a mixture of them is not a measure of the amount of inverted sucrose that is present. To correct the original angle, it is necessary to make an approximate calculation of the amount of inverted sucrose present in the solution before inversion.

The figures obtained with a sample of syrup of rhubarb may be taken as an example of this correction. A 25.5 w/v solution of it gave ${}^{\alpha}{}^{16} = +6.3^{\circ}$ and ${}^{\alpha}{}^{12} = -7.0^{\circ}$. The latter, corrected by equations (2) and (5), became ${}^{10}I^{20} = -6.16$.

The approximate angle of the original inverted sucrose calculated by equation (12) = $0.249 (3.023 \times 6.16 - 6.63) = 3.1^{\circ}$.

This angle (-3.1) is therefore a measure of the inverted sucrose originally present, and can be corrected as usual by equations (2) and (5), which give the value -2.95° . The original angle can then be corrected by the result of this calculation, as the sucrose angle would not be affected by temperature and concentration:

$${}^{10}\alpha^{20} = 6.3 + (3.1 - 2.95) = 6.45^{\circ}.$$

The composition of the original solution can then be calculated by equations (9) and (10):

$$\text{Sucrose} = 0.565 (6.45 + 6.16) = 7.14 \text{ } w/v.$$

$$\text{Original inverted sucrose} = 0.565 (3.023 \times 6.16 - 6.45) = 6.88 \text{ } w/v.$$

As these were 25.5 *w/v* solutions, the syrup contained 28.0 per cent. of sucrose and 26.7 per cent. of inverted sucrose. The latter could be changed to invert sugar by multiplication by 1.05.

REDUCTION.—The following general equation for the calculation of *K*—i.e., reduction expressed as dextrose and lævulose—is sometimes useful :

If “*a*” grm. of sugar or syrup is diluted to “*b*” c.c. = (1),
and “*c*” c.c. of (1) is diluted to “*d*” c.c. by inversion = (2),
and “*e*” c.c. of (2) is diluted to “*f*” c.c. = (3),
and “*g*” c.c. of (3) = 10 c.c. of Fehling solution.

$$(17) K = \frac{5 b d f}{a c e g}.$$

MIXTURES OF SEVERAL SUGARS.—When, in addition to the presence of sucrose, which is more or less inverted, glucose syrup is present, it is necessary to supplement the polarisation figures by a determination of the *K* and the organic solids both before and after fermentation. In such cases it is better to polarise at 20° C. instead of making the complicated temperature correction.

The fermentation may conveniently be performed as follows : Twenty grms. of the substance are weighed and mixed with 220 c.c. of water and 1 grm. of yeast, and the mixture is sterilised by boiling for a short time. After cooling, 3 grms. of yeast are added, and the flask is plugged with cotton-wool and incubated at about 28° C. for three or four days ; 100 c.c. of almost clear liquid are then decanted, and the remainder measured (= “*a*” c.c.). The 100 c.c. are evaporated down to less than one-half, alumina cream added, and diluted to $\frac{10,000}{100+a}$ c.c., so as to give a 20 *w/v* solution. After filtration the solution is analysed. It is a convenience to start two fermentations at once, so that if the *K* of the first indicated that fermentation is incomplete, the second flask can be incubated for a day or two longer, or the turbid liquid residue of the first fermentation may be returned to the incubator.

The following analysis of a sample of war-time “high-class stoneless damson and apple jam” shows the results obtained with such a mixture. The specific rotatory power before inversion was +47.3°, and after inversion +29.3°. These values, calculated by equations (11) and (8), give the specific rotatory power due to sucrose as 13.5°, and showed that 20.3 per cent. of sucrose was present.

	Organic Solids.	<i>K</i> .	[α] _D .
	Per Cent.		
Original	59.3	26	47.3
Subtracting sucrose	20.3	—	13.5
	39.0	26	33.8
After fermentation	16.0	3	24.6
Lost by fermentation	23.0	23	9.2

As the *K* of the fermented portion equalled the organic solids, the latter consisted of dextrose and lævulose. For this fermented sugar [α]_D = $\frac{9.2 \times 100}{23} = 40.4^\circ$.

The percentage composition is then calculated by equation (15) :

$$\text{Invert sugar} = 1.35 (52.8 - 40.4) = 16.8 \text{ per cent.}$$

This shows that 16.8 per cent. of the 23 per cent. (= 3.9 per cent.) of the sugar fermented was invert sugar. The remainder of the *K* (26 - 3.9) may be taken to be dextrose. The optically active part of the 16.0 per cent. of residue after fermentation may be taken to be a mixture of dextrose and dextrin. The specific rotatory power due to the 3 per cent. of dextrose is subtracted.

			Organic Solids.	$[\alpha]_D$.
			Per Cent.	
Unfermented	...	...	16	24.6
Dextrose	...	...	3	1.6
Dextrin, etc.	...	...	13	23.0

$$\text{Dextrin [by equation (8)]} = \frac{100 \times 23}{200} = 11.5 \text{ per cent. This leaves } (13.0 - 11.5) =$$

1.5 per cent. of other unfermented solids.

The complete analysis of the jam was as follows : Sucrose, 20.3; invert sugar, 3.9; dextrose, 22.1; dextrin, 11.5; other soluble organic solids, 1.5; ash, 0.8; insoluble matter, 1.2; and water (by difference), 38.7 = 100.0.

A careful examination of the insoluble matter of the jam only detected 0.04 per cent. of damson skin; so, in addition to being adulterated with glucose syrup, very little damson was present. There was some evidence that the jam had been dyed.

CONSTANTS AND FACTORS FOR SUGARS.

Sugar.	Molecular Weight.	$10[\alpha]_D^{20}$.	<i>B.</i>	<i>C.</i>	<i>c.</i>	<i>D.</i>	<i>d.</i>
Lactose :							
$C_{12}H_{22}O_{11}$...	342.24	55.3°	11.06°	—	—	0.079	0.0015
$C_{12}H_{22}O_{11}, H_2O$...	360.26	52.5°	10.5°	—	—	0.075	0.0014
Maltose :							
$C_{12}H_{22}O_{11}$...	342.24	138°	27.6°	—	—	0.095	0.0007
$C_{12}H_{22}O_{11}, H_2O$...	360.26	131°	26.2°	—	—	0.090	0.0007
Sucrose :							
$C_{12}H_{22}O_{11}$...	342.24	66.5°	13.3°	—	—	0.010	0.0001
Dextrose :							
$C_6H_{12}O_6$...	180.13	52.8°	10.56°	0.030	0.0005	—	—
Lævulose* :							
$C_6H_{12}O_6$...	180.13	95°	19.0°	0.110	0.0006	0.630	0.0066
Invert sugar* :							
$2(C_6H_{12}O_6)$...	360.26	21°	4.2°	0.070	0.0080	0.312	0.0149
Sucrose (inverted)* :							
$C_{12}H_{22}O_{11}$...	342.24	22°	4.4°	0.074	0.0077	0.327	0.0149
Dextrin :							
$n(C_6H_{10}O_5)$...	—	200°	40.0°	—	—	—	—

NOTES

451

$^{10}[\alpha]_D^{20}$ = specific rotatory power of 10 *w/v* solution at 20° C. with sodium flame;
B = rotation of 200 mm. 10 *w/v* solution at 20° C.; *C* = increase in numerical value
 of $^{10}[\alpha]_D^{20}$ for increase of 1 *w/v* of sugar; *c* = concentration coefficient; *D* = decrease
 in numerical value of $^{10}[\alpha]_D^{20}$ for increase of 1° C.; *d* = temperature coefficient;
 * = left-hand rotation.

* * * * *