

# Background elimination in three-dimensional spectroscopy using the intensian method

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The method to eliminate background in the case of quantitative multidimensional spectroscopy, chromatography or any analytical 3-dimensional technique is shown. The 3-dimensional signal is required to be proportional to the concentration of determined substance and the additivity of signals should be obeyed. Eliminated background is assumed to be a low-order polynomial of two variables. The intensian method [1] is a generalization of the Beer–Lambert law, where a certain determinant called *intensian* replaces absorption and absorptivity. In practice there will be no need to use determinants, since usually they are replaced by expressions of few terms. Some details on the practical use of the method are given.

## 1. Introduction

In the last decade a great improvement took place in multidimensional spectroscopy. As yet, this spectroscopy is used in structural (e.g. two-dimensional NMR spectroscopy [2,3]) and qualitative analysis (e.g. GC-MS, LC-UV/vis, GC-IR [4], MultiDimensional GC [5], GC-(Matrix Isolation)-FTIR [6], GC-FTIR-MS [7], GC-(FT-NIR)-(Atomic Emission Spectroscopy) [8,9] and many others). Soon, this technique will come to be routine quantitative spectroscopy and at the same time many problems, well known from commonly used quantitative spectroscopy, will arise.

In the present paper we generalize a formalism of the (2-dimensional) intensian method [1]. We applied this method for determination of  $\Delta H$  and  $\Delta S$  values of the urea-phenol (1 : 1) complex formation [1], and we showed that the method can be competitive to the curve fitting routine. This paper describes how to eliminate one of the most onerous problems of quantitative spectroscopy, the background interference, for the case of 3-dimensional spectroscopy. It is clear that there are many ways to solve this problem. Differentiation of 3-dimensional spectra, spectral background fitting by low-order polynomials of two variables, 3-dimensional band fitting, and filtering with use of a different kind of two-dimensional Fourier

transformations are some of them, which will be certainly used in the field of 3-dimensional spectroscopy. We expect that most of them are just used as an example in the field of optical holography, information theory or electronic signal filtering, but they did not yet diffuse into chemometry, since as we know, until now there are no published chemometric papers describing solutions to this problem.

In this paper we use a Beer–Lambert-like law for 3-dimensional spectroscopy and simple linear functionals (which are in this paper always determinants) acting on 3-dimensional spectral domain. We define those functionals (determinants) as (*3-dimensional*) *intensians* (in contrast to ordinary intensians described earlier [1]). The 3-dimensional intensian in a generalized Beer–Lambert law plays an analogous role as absorption and absorptivity in the ordinary Beer–Lambert law. The intensians possess an important property: they eliminate the background surface and, if it is of a lower degree than the examined three-dimensional band, then a quantitative analysis can be performed. Since determinants are useful in theory but are inconvenient in practice, we have focused on developing some low-order 3-dimensional intensians as expressions of few terms. Knowing some simple properties of intensians, the elimination problem might be reduced to a few operations of multiplications and additions. All presented properties of 3-dimensional intensians have been derived based on the fundamental knowledge about determinants [10] and analytic geometry [11]. However, in our opinion, using any computer program in calculating determinants (of order up to ca.  $7 \times 7$ ) and imitating the scheme shown in the model example, one can use the 3-dimensional intensian method based only on the generalized Beer–Lambert law and the structure of the 3-dimensional intensian.

## 2. Theory

Assume that the intensity  $A(x, y)$  of a selected 3-dimensional spectral band of a substance is directly proportional to its concentration  $c$ , namely the Beer–Lambert law for the (chosen) 3-dimensional band is valid:

$$A(x, y) = a(x, y) \cdot b \cdot c, \quad (1)$$

where

$x, y$  = IR, GC, UV, NMR, or other spectroscopic scale,

$b$  = path length (or other measurement factor),

$c$  = concentration,

$a(x, y)$  = intensity for  $b, c = 1$  (absorptivity),

$A(x, y)$  = intensity (absorption).

Let us assume, that the unknown background  $B(x, y)$ , which interferes with the band of interest  $A(x, y)$ , can be described as a polynomial (of two variables) of a

degree that does not exceed certain positive integer  $k$ , whereas  $A(x, y)$  can be expanded in a power series (of two variables) of a degree not less than  $k + 1$ :

$$B(x, y) = \sum_{0 \leq i+j \leq k} \beta_{ij} x^i y^j, \tag{2}$$

$$A(x, y) = \sum_{i,j=0}^{\infty} \alpha_{ij} x^i y^j, \quad \exists i, j: \quad i + j \geq k + 1, \quad \alpha_{ij} \neq 0.$$

Moreover, let us assume that spectrum  $S(x, y)$  (observed in a selected region) is a sum of  $A(x, y)$  and  $B(x, y)$ :

$$S(x, y) = A(x, y) + B(x, y). \tag{3}$$

Now using any linear functional  $\mathcal{F}$  (assigning a value to a function of two variables) we can express the Beer–Lambert law (1) in terms of  $\mathcal{F}$ :

$$\mathcal{F}(A(x, y)) = \mathcal{F}(a(x, y) \cdot b \cdot c) = b \cdot c \cdot \mathcal{F}(a(x, y)). \tag{4}$$

Additivity of spectra is kept in force by such a functional too:

$$\mathcal{F}(S(x, y)) = \mathcal{F}(A(x, y) + B(x, y)) = \mathcal{F}(A(x, y)) + \mathcal{F}(B(x, y)). \tag{5}$$

We intend here to describe a linear functional satisfying the following condition:

$$\mathcal{F}(B(x, y)) \equiv 0 \quad \text{while} \quad \mathcal{F}(A(x, y)) \neq 0. \tag{6}$$

The linear functional fulfilling eq. (6) is named by us (*3-dimensional intension*). It is not difficult to verify that the following determinant possesses the desired properties:

$$J^{3\text{-dim}}(f(x, y)) = \begin{vmatrix} f(x_1, y_1) & f(x_2, y_2) & \dots & f(x_m, y_m) \\ 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_m \\ y_1 & y_2 & \dots & y_m \\ x_1^2 & x_2^2 & \dots & x_m^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^i y_1^j & x_2^i y_2^j & \dots & x_m^i y_m^j \end{vmatrix}, \tag{7}$$

where

$0 \leq i + j \leq k =$  degree of polynomial  $B(x, y)$ ,

$f(x_l, y_l)$  = value of  $f(x, y)$  at point  $(x_l, y_l)$ ,

$x_l, y_l$  = value of arguments  $x$  and  $y$ ,

$(x_l, y_l) \neq (x_p, y_p)$  for  $l \neq p$ ,

$f(x, y)$  denotes  $A(x, y), B(x, y)$  or  $S(x, y)$ .

Note that generally the order  $m \times m$  of the intension (7) should not be lower than that which results from degree  $k$  of the background to be eliminated (e.g.  $m \geq 0.5(k+1)(k+2)+1$ ). However, if one knows that a particular monomial term is absent in the background formula, then the order of the intension might be reduced.

It is worth noticing that in practice intensions will be used in their form (8) expanded according to the elements of the first row and their cofactors:

$$J^{3-\dim}(f(x, y)) = \sum_{i=0}^s d_i f(x_i, y_i), \quad (8)$$

where  $d_i$  are cofactors of  $f(x_i, y_i)$ .

We shall term signed minors  $d_i$  as *intension coefficients*.

### 3. Model example of use of a 3-dimensional intension

For simplicity, an example will be given in cases where a 3-dimensional spectral band  $A(x, y)$  is interfered by a background plane  $B(x, y)$ . Let us imagine that we perform a GC-IR quantitative analysis and that we determine a certain ester (component of complex mixture) based on its C=O stretching vibration band. Let the 3-dimensional band of this ester for standard conditions ( $c = 1, b = 1$ ) be of a Lorentzian shape:

$$a(x, y) = 0.9(1 + [(1730 - x)/5]^2 + [(100 - y)/2]^2)^{-1},$$

where

$x$  = IR abscissa,

$y$  = GC abscissa,

(1730, 100) = maximum abscissa,

0.9 = intensity in maximum,

5 = half of the band width in intersection perpendicular to the IR abscissa,

2 = half of the band width in intersection perpendicular to the GC abscissa.

(1) Let us calculate a 3-dimensional 4-point intension for standard conditions. First, we select four points, e.g. (1730, 100); (1740, 102); (1735, 100); (1725, 98). Next, note that those points are placed at vertices of the parallelogram. Thus from property (a) of 4-point intension properties (see section 5), we know that intension coefficients have equal absolute values and that the signs of coefficients for adjacent vertices are opposite. Therefore, we can put  $\pm 1$ , since we can multiply both sides of the generalized Beer-Lambert law by a nonzero number. Then,

$$\begin{aligned} \mathcal{J}_4^{3-\dim}(a(c, y)) &= a(1730, 100) - a(1740, 102) + a(1735, 100) - a(1725, 98) \\ &= 0.90 - 0.15 + 0.45 - 0.30 = 0.90. \end{aligned}$$

(2) Let the background in the region of interest be described by the plane

$$B(x, y) = 0.001x + 0.005y - 22.000.$$

If the concentration of our ester in the analysed mixture is 0.7, then the contributions of the ester spectrum and background spectrum at the selected points are as follow:

$$A(1730, 100) = 0.630; \quad B(1730, 100) = 0.30;$$

$$A(1740, 102) = 0.105; \quad B(1740, 102) = 0.50;$$

$$A(1735, 100) = 0.315; \quad B(1735, 100) = 0.35;$$

$$A(1725, 98) = 0.210; \quad B(1725, 98) = 0.15;$$

and the intensities of the spectrum  $S(x, y)$  at the selected points are as follow:

$$S(1730, 100) = 0.630 + 0.30 = 0.930;$$

$$S(1740, 102) = 0.105 + 0.50 = 0.605;$$

$$S(1735, 100) = 0.315 + 0.35 = 0.665;$$

$$S(1725, 98) = 0.210 + 0.15 = 0.360.$$

(3) Now we calculate the 4-point intensian of the spectrum  $S(x, y)$ :

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = 0.930 - 0.605 + 0.665 - 0.360 = 0.630.$$

(4) We calculate the concentration of the substance from the generalized Beer–Lambert law (for  $b = 1$ ):

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = \mathcal{J}_4^{3-\dim}(a(x, y)) \cdot c \cdot b,$$

then, since  $b = 1$ , we obtain

$$c = \frac{\mathcal{J}_4^{3-\dim}(s(x, y))}{\mathcal{J}_4^{3-\dim}(a(x, y))} = \frac{0.63}{0.90} = 0.7.$$

Notice that the same result will be obtained for any background plane. So, we do not need to know nor estimate the plane equation in contrast to background approximation methods.

#### 4. General properties of 3-dimensional intensians

The intensian (7) as a determinant of a matrix is linear with respect to each of its row, thus we have

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = \mathcal{J}_4^{3-\dim}(A(x, y)) + \mathcal{J}_4^{3-\dim}(B(x, y)). \quad (9)$$

Since the background  $B(x, y)$  is of degree  $\leq k$ , then the first row of  $J^{3-\dim}(B(x, y))$  is linearly dependent on the remaining rows and this intension vanishes. Linear dependence of the rows of a determinant  $J^{3-\dim}(B(x, y))$  is a fundamental theoretical reason why the method performs well.

At the same time, since the band of interest,  $A(x, y)$ , is a function of degree  $\geq k + 1$ , therefore  $J^{3-\dim}(A(x, y))$  is equal to zero only in some special situations.

Hence we have

$$J^{3-\dim}(S(x, y)) = J^{3-\dim}(A(x, y)) = bcJ^{3-\dim}(a(x, y)). \quad (10)$$

We can ignore the background  $B(x, y)$  and perform a quantitative analysis as in the case of classical 1-dimensional spectrometrical analysis.

$J^{3-\dim}(a(x, y))$  plays the same role in formula (9) as the absorptivity in the ordinary Beer–Lambert law.

Now we describe some additional properties of the intension (7) which ought to be taken into consideration when intensions are put into practice.

(i) If the points  $(x_i, y_i, S(x_i, y_i))$  of the examined spectrum  $S(x, y)$  are on the surface describable by a linear combination of monomials to be found in the matrix (7), then the intension is singular.

(ii) If  $n - 1$  out of  $n$  points  $(x_i, y_i)$  are on a curve (in  $XY$  plane) describable by a linear combination of monomials as above, then one of the intension coefficients is singular and the surface of the desired degree cannot be eliminated. For example,  $n - 1$  out of  $n$  points cannot have a form  $(x_i, \alpha x_i + \beta)$ , where  $\alpha$  and  $\beta$  are any numbers.

(iii) The Cartesian coordinates  $XYZ$  of a registered spectrum can be arbitrarily translated by the vector  $[a, b, c]$  ( $a, b, c$  any numbers), which leaves the intension unaltered. Thus, we can always set up the origin of coordinates at any point.

(iv) If the determinant (7) is of order  $k \times k$ , where  $k = 0.5(n^2 + 3n + 4)$  for  $n = 0, 1, \dots$  (e.g.  $k = 2, 4, 7, 11, \dots$ ), and every monomial of the degree that does not exceed  $n$  appears in the appropriate row of the matrix, then any rotation about the  $z$  axis leaves the intension unchanged. In those cases we can use any isometry of the plane  $XY$  to choose the position of coordinates.

(v) For intensions defined as in (iv) the general Laplace expansion of a determinant enables us to find an expression for the intensions, coefficients; however, an explicit form of these coefficients is rather complicated.

(vi) The maximal absolute measurement error of an intension can be expressed by

$$\Delta(J^{3-\dim}(f(x, y))) = \sum_{i=0}^s |d_i| \Delta(f(x_i, y_i)), \quad (12)$$

where  $\Delta(f(x, y))$  is the error connected with either the position error or the intensity error.

(vii) A more detailed analysis of the error in the intension value should be based on an examination of noise distribution functions in neighbourhoods of  $S(x_i, y_i)$ .

If by  $r_i$  we denote a random variable, defined as the difference between the measured and the mean intensity at point  $(x_i, y_i)$ , and by  $G(r_i)$  its distribution function, then the distribution function of a new random variable  $R$  is defined as

$$R = \sum_{i=0}^s d_i r_i, \tag{13}$$

where  $d_i$ , the intensian coefficient, is a product of functions  $G(d_i r_i)$ , since  $r_i$  are supposed to be independent. Furthermore, if  $G(r_i) = G(r)$  for  $i = 1, 2, \dots, s$  and  $G(r)$  is a normal distribution, then

$$G(R) = \left( \sum_{i=0}^s d_i \right)^{-0.5} G(r). \tag{14}$$

Since in practice rather lower-order intensians will be used, we can, therefore, now mention some more useful properties of intensians of order 4 and additionally some remarks on order 7.

First, it should be noticed, that 4- and 7-point intensians fulfil the requirements of (iv), thus, for those intensians one can select an optimal set of rectangular coordinates  $XY$ . For 5- and 6-point intensians, condition (iv) is not valid and their values depend on the angle of rotation about the  $z$  axis.

### 5. Lower-order 3-dimensional intensians

The 4-point (3-dimensional) intensian has the form

$$J_4^{3\text{-dim}}(S(x, y)) = \begin{vmatrix} S_1 & S_2 & S_3 & S_4 \\ 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \end{vmatrix}, \tag{15}$$

where  $S_i = S(x_i, y_i)$ ,  $i = 1, 2, 3, 4$ .

Based on (i) we have to preclude such arrangements of  $S_i$  to be placed on any plane ( $z = \alpha x + \beta y + \gamma$ ;  $\alpha, \beta, \gamma$  any numbers).

From (ii) we know that any three points out of four cannot be positioned on a straightline in the  $XY$  plane.

From (iii) and (iv) we know that for any distribution of points  $(a_1, b_1), (a_2, b_2), (a_3, b_3), (a_4, b_4)$  we can choose  $XY$  coordinates to obtain the following set of points:  $(0, 0), (0, y_1), (x_2, y_2), (x_3, y_3)$ . Then

$$J_4^{3\text{-dim}}(S(x, y)) = S(0, 0) \cdot (x_2 y_3 - y_1) - x_3 (y_2 - y_1) - S(0, y_1) \cdot (x_2 y_3 - x_3 y_2) - S(x_2, y_2) \cdot y_1 x_3 + S(x_3, y_3) \cdot y_1 x_2. \tag{16}$$

If points  $(x_i, y_i)$  are placed at the vertices of an arbitrary:

(a) *Parallelogram*, then the absolute values of  $d_i$  are equal to the product of the lengths of the parallelograms sides. The sign for adjacent vertices is opposite. Additionally, the rectangular arrangement of points eliminates any function symmetrical with respect to the rectangular axis of symmetry.

(b) *Trapezoid*, then  $d_i$  depends only on the length of its bases  $a$  and  $b$  and altitude  $h$ . Thus, for this trapezoid  $((0, 0), (h, y_1), (h, y_1 + b), (0, a))$  we have

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = h[b(S(0, 0) - S(0, a)) + a(S(h, y_1 + b) - S(h, y_1))]. \quad (17)$$

(c) *Deltoid*  $((-a, 0), (a, 0), (0, b), (0, c))$ , then

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = a[(b - c)(S(-a, 0) + S(a, 0)) + 2(S(0, b)c - S(0, c)b)]. \quad (18)$$

(d) *Quadrilateral* with one right angle  $((0, 0), (a, 0), (0, b), (c, d))$ , then

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = S(0, 0)(ab - bc - ad) + S(a, 0)bc + S(0, b)ad - S(0, c)ab. \quad (19)$$

(e) If three points are placed on the vertices of an equilateral triangle and the fourth at an arbitrary position, then we can set  $b$  equal to  $3^{0.5}a$  in the above formula. If the fourth point is placed at the centroid of this triangle, then,

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = (2/3)3^{0.5}a^2[3S(0, 3^{0.5}/3) - S(-a, 0) - S(0, a) - S(0, c)]. \quad (19')$$

The above formula (19') seems to be optimal for a symmetrical band with its maximum placed at the centroid of the equilateral triangle, since the coefficient for this point is three times larger than for the other points.

(f) Finally, if  $y_i = \alpha x_i + \beta x + \gamma$  ( $\alpha, \beta, \gamma$  any numbers), then

$$\mathcal{J}_4^{3-\dim}(S(x, y)) = \sum_{i=1}^4 S(x_i, y_i)(-1)^{i+1} \prod_{\substack{1 \leq k < j \leq 4 \\ k, j \neq i}} (x_j - x_k). \quad (20)$$

For an elimination of any background of second degree one needs to use the 7-point intensian.

The 7-point intensian has form

$$\mathcal{J}_7^{3-\dim}(S(x, y)) = \begin{vmatrix} S_1 & S_2 & S_3 & S_4 & S_5 & S_6 & S_7 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 \\ y_1 & y_2 & y_3 & y_4 & y_5 & y_6 & y_7 \\ x_1^2 & x_2^2 & x_3^2 & x_4^2 & x_5^2 & x_6^2 & x_7^2 \\ x_1 y_1 & x_2 y_2 & x_3 y_3 & x_4 y_4 & x_5 y_5 & x_6 y_6 & x_7 y_7 \\ y_1^2 & y_2^2 & y_3^2 & y_4^2 & y_5^2 & y_6^2 & y_7^2 \end{vmatrix}, \quad (21)$$



where  $S_i = S(x_i, y_i)$ .

Any rotation or translation of  $XY$  coordinates does not perturb this 7-point intensionian.

If we choose the  $(0, 0)$  point as one of the seven points  $((0, 0), (x_1, y_1), \dots, (x_6, y_6))$  then the general expression for 7-point intensionian coefficients has the form

$$d_i = \sum (-1)^{J+K+L} d_{jkl} D_{mnp}, \tag{22}$$

where  $0 \leq i \leq 6; j, k, l \neq i; 0 \leq j < k < l \leq 6; m, n, p \neq i, j, k, l; m < n < p, J = j$  if  $j < i$  and  $j + 1$  if  $j > i$ , similarly for  $K$  and  $L$ .

$$d_{jkl} = (x_j y_k - y_j x_k)(x_j y_l - y_j x_l)(x_k y_l - y_k x_l)$$

$$D_{mnp} = (x_m y_n - y_m x_n)(x_m y_p - y_m x_p)(x_n y_p - y_n x_p)$$

The sum for  $d_0$  is composed of 20 terms and for the other coefficients, 10 terms, since  $D_{0jk} = 0$  for  $j, k = 1, \dots, 6$ .

The choice of the arrangement of points to build a nonvanishing 7-point intensionian is not an easy problem. Generally, the row  $S(x_i, y_i)$  cannot be a linear combination of other rows of 7-point intensionian (21).

If our analyzed band has one maximum then it is natural to choose one point in this maximum and the other points around it. Therefore, however, it is very probable that such an intensionian will be vanishing. For example, if the points are chosen on the vertices and in the middle (point  $(0, 0)$ ) of a regular hexagon, then for a function of two variables symmetrical with respect to the  $(0, 0)$  point (e.g.  $\exp(x^2 + y^2)$ ), the intensionian vanishes. It is important to notice that the most significant  $(0, 0)$  coefficient vanishes if six points are at the vertices of a convex hexagon with its sides parallel in pairs.

As an example we show one particular, simple solution to this problem. If the points are chosen from the following set of points  $((0, 0), (c, 0), (-c, 0), (0, b), (0, -b), (a, a), (a, -a))$ , then

$$\begin{aligned} J_7^{3-\dim}(S(x, y)) &= S(0, 0)8a^2bc(a^2b^2 + a^2c^2 - c^2b^2) - S(c, 0)4a^3b^3c)a + c \\ &\quad + S(-c, 0)4a^3b^3c(-a + c) - S(0, b)4c^3a^4b - S(0, -b)4c^3a^4b \\ &\quad + S(a, a)4a^2b^3c^3 + S(a, -a)4a^2b^3c^3. \end{aligned}$$

If the above formula is divided by  $a^3b^3c^3$  then it has the simpler form

$$\begin{aligned} J_7^{3-\dim}(S(x, y)) &= S(0, 0)8(-1/a + a/c^2 + a/b^2) - S(c, 0)4(a/c^2 + 1/c) \\ &\quad + S(c, 0)4(-a/c^2 + 1/c) - S(0, b)4a/b^2 - S(0, -b)4a/b^2 \\ &\quad + S(a, a)4/a + S(a, -a)4/a. \end{aligned}$$

If an analyzed band is not a symmetrical one, or if there is any other reason to chose points not as regular as in the above example, then one should try various sets of points to maximize the intensionian value.

With increasing order of the intensian, not only does the computation of coefficients become more arduous, but also it is more difficult to arrange points to be not describable by a linear combination of monomials from the intensian.

## 6. Concluding remarks

In this paper we have formulated a general solution for the background elimination in the case of 3-dimensional spectroscopy. We described more important properties of the general solution and particular solutions for the elimination of any plane and background of the second degree.

The intensian method can easily be applied in laboratory practice, since a standard determinant calculation program can be used for its applications.

Using the intensian method we do not need to know nor estimate the background equation and it is enough to know (or assume) its order. If the background degree is assumed correctly then the concentrations of a sample obtained, based on two different intensians, are the same.

If there is a need to eliminate a noise then an arithmetic mean of intensians can be applied, since it is an intensian taken for arithmetic means of points [1].

It should be noted here that any background surface interfering with a 3-dimensional band might be eliminated using ordinary (intensian) methods of background elimination for (two) intersections of a 3-dimensional band. Such a solution has, however, an important weakness – it always requires more measurements than in an adequate 3-dimensional method and, as a consequence, has a larger influence of noise. For example, to eliminate any plane we need to measure the signal intensity in four points, whereas the 2-dimensional intensian method offers us measurements in 6 points, three for each intersection.

We showed that the 2-dimensional intensian method was competitive to the band fitting procedure [1] but certainly less complicated in use. We expect that the same will hold true for the 3-dimensional intensian method.

Finally, it is quite easy to generalize the intensian method for more than 3-dimensional spectroscopy, but first the 3-dimensional version should be carefully tested in practice.

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## Index of used symbols

$x, y$       UV, IR, GC, NMR or other scale,

$A(x, y)$	intensity (absorption) of the 3-dimensional band of interest,
$a(x, y)$	standard intensity (absorption) of the 3-dimensional band of interest,
$B(x, y)$	intensity (absorption) of 3-dimensional background,
$S(x, y)$	intensity (absorption) of 3-dimensional multicomponent spectrum,
$f(x, y)$	auxiliary function: $f(x, y) = A(x, y), B(x, y), a(x, y), S(x, y)$ ,
$(x_i, y_i)$	selected point, $i$ positive integer number,
$f(x_i, y_i)$	value of $f(x, y)$ in point $(x_i, y_i)$ ,
$S_i$	value of $S(x, y)$ in point $(x_i, y_i)$ ,
$b$	pathlength, measurement coefficient,
$c$	concentration,
$\alpha, \beta, \gamma, \delta$	real numbers,
$\alpha_{ij}, \beta_{ij}$	real coefficients of power expansions,
$x^i y^j$	monomial of degree $(i + j)$ ,
$\mathcal{F}(\cdot)$	linear functional acting on 3-dimensional spectral functions,
$\mathcal{J}^{3-\text{dim}}(\cdot)$	3-dimensional intension acting on 3-dimensional spectral functions,
$\mathcal{J}_n^{3-\text{dim}}(\cdot)$	3-dimensional $n$ -points intension,
$d_i$	$i$ th intension coefficient, cofactor of expansion of $\mathcal{J}_n^{3-\text{dim}}(f(x, y))$ according to its first row (eq. (10)),
$\Delta(\cdot)$	absolute error,
$r_i, R$	random variables: eqs. (13) and (14),
$G(\cdot)$	(normal) distribution function,
$z$	ordinate axis,
$a - f, h$	abbreviations for some arguments,
$d_{ijk}, D_{mnp}$	abbreviations defined in eq. (22).

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