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A method based on the DAOSD approach to estimate the variation of the peak position and bandwidth caused by intermolecular interactions

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HIGHLIGHTS

- Under intermolecular interaction, peak position, bandwidth may change simultaneously.
- Change on both peak position and bandwidth will produce butterfly cross peaks.
- A method is set up to estimate change of peak position, bandwidth from cross peaks.
- The validity of the approach is confirmed by computer simulation.

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ABSTRACT

Subtle spectral variations caused by intermolecular interactions, which are hardly observed in the original one-dimensional spectra or the second derivative spectra, can be distinctly visualized via spectral patterns in two-dimensional spectra generated by using double asynchronous orthogonal sample designed scheme (DAOSD). If intermolecular interaction only brings about band-shift on a characteristic peak, a pair of cross peaks appears in the corresponding near diagonal region. If intermolecular interaction induces variation of bandwidth only, a cluster of cross peaks forms a diamond pattern in the near diagonal region. In both cases, the variation of peak position or bandwidth can be deduced quantitatively from the pattern of cross peaks. If intermolecular interaction causes variations on both peak position and bandwidth, four cross peaks form a butterfly pattern. In this case, however, it is not straightforward to estimate the variation of peak position and bandwidth directly from the patterns of the cross peaks. In this paper, we propose an algorithm to estimate the variations of peak position and bandwidth of a characteristic peak caused by intermolecular interactions. The validity of this approach was confirmed by computer simulation on several model systems.

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1. Introduction

Intermolecular interactions, which influence the arrangement, orientation and conformations of molecules, play a crucial role in many physical, chemical and biological processes, including assembly of supra-molecular architectures [1–5], molecular recognition [6,7], and molecular catalysis [8]. Spectroscopic methods are very important in characterizing such intermolecular interactions [9–11].

In many cases, however, intermolecular interactions can only induce subtle spectral changes. Consequently, the following problem poses a great challenge to the investigation of intermolecular interactions by using spectroscopic method.

In a typical chemical system, a substance (P) whose characteristic peak at X_P is shown as trace 1 in Scheme 1 is involved in intermolecular interaction. Under intermolecular interaction, a small fraction of P undergoes subtle structural variation and converts

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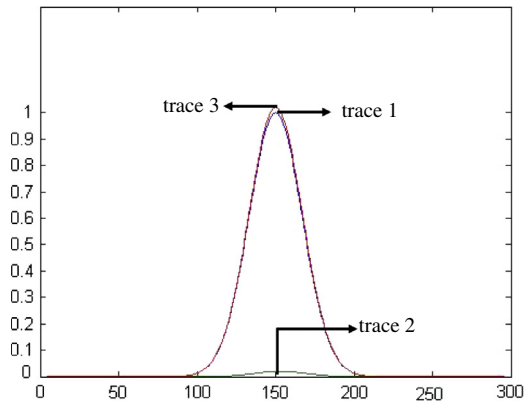


Scheme 1. Characteristic band of P (trace 1). Under intermolecular interaction, a small fraction of P undergoes subtle structural variation and converts into a new species (U), the characteristic peak of U is shown as trace 2. In experiment, only the summation spectrum of P and U (trace 3) is observable. From trace 3, it is impossible to retrieve spectra of U even if resolution enhancement technique is used.

into U (the spectrum of U is illustrated as trace 2 in Scheme 1). Comparing with the spectrum of P, the variation of peak position of U is quite small. Consequently, severe band overlapping occurs between the peak of P and peak of U. Furthermore, the intermolecular interaction is often quite weak and the content of U is rather low. Hence, the spectrum of U is overwhelmed by that of P. In spectroscopic experiment, the summation of trace 1 and trace 2 (trace 3 in Scheme 1) can only be observed. In this situation, it is difficult to reveal existence of the spectrum of U from trace 3 even if resolution enhancement techniques, such as second derivative spectra, are utilized.

The advent of 2D correlation spectroscopy [12–15] provides a new avenue to characterizing intermolecular interactions. There are many progresses on the studies of intermolecular interaction by using 2D spectroscopic methods reported in the literature over the past two decades [16–27]. In our previous work, we have introduced orthogonal sample design scheme (OSD) approach that provides an unambiguous relationship between the cross peak in 2D synchronous spectrum and intermolecular interaction [28–32]. Moreover, we have refined this approach by introducing asynchronous orthogonal sample design (AOSD) [33–35] and double orthogonal sample design (DOSD) schemes [36] to enhance the ability of the 2D correlation spectroscopy to characterize spectral behaviors among solutes under intermolecular interactions.

Further studies show that 2D asynchronous spectra generated by using the OSD, DOSD, and AOSD approaches serve as a new spectral resolution enhancement method [28–36]. Considering the afore-mentioned system, we have demonstrated that cross peaks around (X_P,X_P) in 2D asynchronous spectrum generated by using AOSD and DOSD approach are very useful in revealing severely overlapped sub-band:

(1) If intermolecular interaction only brings about band-shift on the characteristic peak of P, a pair of cross peaks that are anti-symmetric about the diagonal can be observed around (X_P,X_P) in the 2D asynchronous spectrum generated by using AOSD and DOSD approaches [32,36]. The sign of the cross peaks can be used to determine whether the peak undergoes red-shift or blue-shift. Moreover, the magnitude of band-shift can be calculated based on the peak position of the cross peak in 2D asynchronous spectrum.
(2) If intermolecular interaction only induces change on bandwidth, a diamond-shape cross peak cluster composed of a pair of horizontal cross peaks and a pair of vertical cross peaks appear in the resultant 2D asynchronous spectrum. The sign of the cross peaks can be used to determine whether the bandwidth increases or decreases. A method to estimate the variation of bandwidth has also been established [36].

In many cases, however, intermolecular interactions may render peak position, bandwidth, and absorptivity of the corresponding characteristic peaks to change simultaneously. As a result, the spectral patterns of 2D spectra generated by using OSD, DOSD, and AOSD approaches become too complicated to reveal how peak position, bandwidth, and absorptivity change under intermolecular interaction. This problem prevents us from getting further information on the physico-chemical nature of the intermolecular interactions. Recently, we proposed a new approach called "double asynchronous orthogonal sample design scheme" approach (DAOSD) to resolve the problem [37]. This approach produces a pair of complementary sub-2D asynchronous so that the spectral patterns are significantly simplified. Computer simulation results demonstrated the variation of peak position, bandwidth and absorptivity of a characteristic peak can be deduced at a qualitative level (increase, invariant, decrease) via the spectral patterns of the cross peaks generated by using 2D asynchronous spectra. However, estimation on the extent of variation of peak position and bandwidth when both peak position and bandwidth change simultaneously is still an unsolved problem. In this paper, we present an approach to address this problem.

2. The model system

To simulate intermolecular interaction between P and Q, we assume that part of P undergoes subtle structure variation and converts into U and part of Q converts into V under intermolecular interaction. This could be specified in terms of Eq. (1) and the strength of intermolecular interaction can be characterized by the corresponding equilibrium constant K.

$$\mathrm{P} + \mathrm{Q} \overset{K}{\rightleftarrows} \mathrm{U} + \mathrm{V} \tag{1}$$

The K value of Eq. (2) is set as 0.01 in this paper.

The spectral function of each substance (P, Q, U and V) possesses only one characteristic peak. The peak function for each substance is represented by a Gaussian function as shown in Eq. (2).

$$f_j(x) = \varepsilon_j L e^{-\ln 2 \frac{(x-x_j)^2}{w_j^2}} \tag{2}$$

where W_j, X_j, and ε_j are the bandwidth, peak position, and absorptivity of the characteristic band of the jth chemical species. Here j stands for P, Q, U and V). L is the path-length and is set as 1 for convenience.

The spectral function of a 1D spectrum for a solution is the summation of the peak function of P, Q, U and V as shown in Eq. (3).

$$A(x) = C_P^{eq} f_P(x) + C_Q^{eq} f_Q(x) + C_U^{eq} f_U(x) + C_V^{eq} f_V(x) \tag{3}$$

where $f_P(x)$, $f_Q(x)$, $f_U(x)$ and $f_V(x)$ are spectral functions of P, Q, U and V. C_P^{eq}, C_Q^{eq}, C_U^{eq} and C_V^{eq} are equilibrium concentrations of P, Q, U and V. The equilibrium concentrations of P, Q, U and V can be calculated by using the initial concentrations of P and Q and the equilibrium constant K.

3. Brief description of the DAOSD approach

The basic theory and spectral properties of asynchronous spectra generated by using the DAOSD approach is described in our previous paper [37]. Herein we just give only a brief description on the DAOSD approach.

The aim of the DAOSD approach is to investigate intermolecular interaction between two solutes (denoted as P and Q here) dissolved in the same solutions. A characteristic peak of P and a characteristic peak of Q are utilized to reflect intermolecular interaction. The peak position of P and Q are X_P and X_Q, respectively. The characteristic peaks of P and Q are not overlapped. In addition, the contributions from the solvent to the two characteristic peaks mentioned above do not occur. In the DAOSD approach, two groups of solutions are prepared and the initial concentrations of P and Q are selected as the requirement of the DAOSD approach shown in Eq. (4).

Group 1:

$$\vec{\mathbf{C}}_P = \begin{bmatrix} s \\ \cdots \\ s \\ \cdots \\ s \end{bmatrix} \qquad \vec{\mathbf{C}}_Q = \begin{bmatrix} C_Q^1 \\ \cdots \\ C_Q^i \\ \cdots \\ C_Q^n \end{bmatrix} \tag{4a}$$

Group 2

$$\vec{\mathbf{C}}_P = \begin{bmatrix} C_P^1 \\ \vdots \\ C_P^i \\ \vdots \\ C_P^n \end{bmatrix} \qquad \vec{\mathbf{C}}_Q = \begin{bmatrix} t \\ \vdots \\ t \\ \vdots \\ t \end{bmatrix} \tag{4b}$$

where s and t are constant values that are set arbitrarily.

For any $i, j \in \{1, \ldots, n\}$, if $i \neq j$, $C_P^i \neq C_P^j$, and $C_Q^i \neq C_Q^j$.

According to the algorithm proposed by Noda [15], an asynchronous spectrum, denoted as $\Psi_P(x,y)$, is constructed based on the 1D spectra of the solutions from Group 1. Another 2D asynchronous spectrum, denoted as $\Psi_Q(x,y)$, is generated via the 1D spectra of the solutions of Group 2. That is to say, 2D asynchronous correlation spectrum is constructed according to Eq. (5).

$$\Psi(x,y) = \frac{1}{n-1}\vec{\tilde{\mathbf{A}}}^T(x)\mathbf{N}\vec{\tilde{\mathbf{A}}}(y) \tag{5}$$

where T stands for transposition, n is the number of solutions used to construct the 2D asynchronous spectrum, and $\mathbf{N}$ is the Hilbert–Noda transformation matrix. All the calculations are based on a program written in our lab by using a software of MATLAB (The Math Works Inc.).

The advantage of the DAOSD approach is that variation of peak position, bandwidth and absorptivity of the characteristic peaks of P and Q are manifested in separated spectral regions:

In $\Psi_P(x,y)$, cross peaks around (X_Q,X_Q) contain valuable information about the variation of peak position and bandwidth of the characteristic peak of Q. Cross peaks around (X_P,X_Q) and (X_Q,X_P) consist of valuable information about variation of peak position, bandwidth and absorptivity of the characteristic peak of P. In $\Psi_Q(x,y)$, cross peaks around (X_P,X_P) contain valuable information about the variation of peak position and bandwidth of the characteristic peak of P; cross peaks around (X_P,X_Q) and (X_Q,X_P) contain valuable information about variation of peak position, bandwidth and absorptivity of the characteristic peak of Q.

The above spectral feature of the 2D asynchronous spectra generated by using the DAOSD approach makes it possible to study the variation of peak position and bandwidth at quantitative level.

4. Results and discussion

According to the mathematical properties of the DAOSD approach, the spectral pattern of cross peaks (including the number of cross peaks and peak position) around (X_P,X_P) in Ψ_Q is only related to X_P, W_P, X_U and W_U. Thus, it is expected that X_U and W_U can be obtained based on the information contained in the cross peaks around (X_P,X_P) in Ψ_Q. In the following part, we focus on cross peak around (X_P,X_P) in Ψ_Q to explore if it is possible to estimate the values of X_U and W_U.

Here we define the variation of peak position and bandwidth as follows:

$$\begin{aligned} \Delta X_P &= X_U - X_P \\ \Delta W_P &= W_U - W_P \end{aligned} \tag{6}$$

When both ΔX_P and ΔW_P are non-zero, a typical $\Psi_Q(x,y)$ is shown in Fig. 1. Around (X_P,X_P), four cross peaks form a butterfly pattern. The projections of extreme point of the four cross peaks are marked as peak A, B, C and D and the coordinates of A, B, C and D are x_A, y_A, x_B, y_B, x_C, y_C, x_D, and y_D.

Computer simulations demonstrated that the changes of ΔX_P and ΔW_P bring about corresponding changes of the peak positions of the four cross peaks. Thus, ΔX_P and ΔW_P can be expressed as functions of x_A, y_A, x_B, y_B, x_C, y_C, x_D, and y_D. However, peak A and D are anti-symmetric about the diagonal. Similarly, peak B and C are anti-symmetric about the diagonal. Consequently, there are only two independent cross peaks with four useful spectral coordinates. Thus, ΔX_P and ΔW_P are expressed as functions of x_A, y_A, x_B, and y_B.

Herein two functions (f_a and f_b) are established. On one hand, f_a and f_b are functions of ΔX_P and ΔW_P. On the other hand, the values of $f_a(\Delta X_P, \Delta W_P)$ and $f_b(\Delta X_P, \Delta W_P)$ are functions of x_A, y_A, and x_B as shown in Eq. (7).

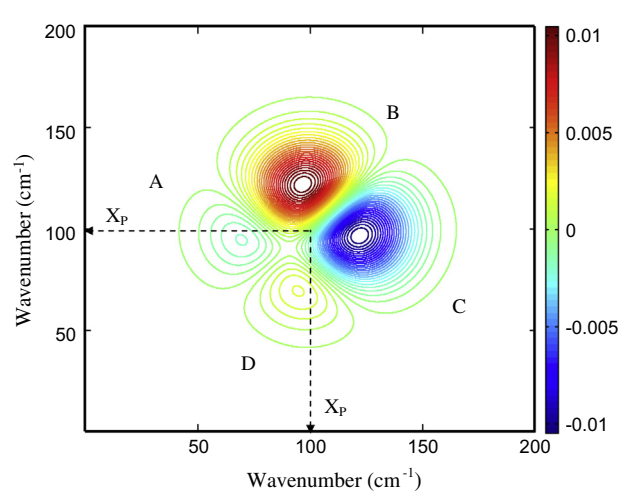


Fig. 1. Typical 2D asynchronous spectrum (Ψ_Q) generated by using the DAOSD approach. The cross peaks form a butterfly pattern when both ΔX_P and ΔW_P are non-zero.

Table 1
Initial concentration series of P and Q in the model system. The concentration series meet the requirement of the DAOSD approach to generate Ψ_Q.

Sequence number	C_P^{init} (mL/mL)	C_Q^{init} (mL/mL)
1	1.00	5.00
2	2.00	5.00
3	8.00	5.00
4	9.00	5.00

Table 2
Spectral variables of the chemical species P, Q, U and V in the model system where the bandwidth and peak position of U are varied.

Spectral variable	Peak position (cm^{-1})	Bandwidth (cm^{-1})	Absorptivity
P	100	20	1.0
Q	400	20	1.0
V	400	20	1.0

$$f_a(X_U, W_U) = f_1(\Delta X_P, \Delta W_P) = g_a(x_A, y_A, x_B) = x_A + y_A + x_B + y_B \quad (7a)$$

$$f_b(X_U, W_U) = f_1(\Delta X_P, \Delta W_P) = g_b(x_A, y_A, x_B) = x_A + y_A - x_B - y_B \quad (7b)$$

For a specific chemical system, the X_U, W_U have definite values. On the other hand, the peak positions of cross peaks around (X_P,X_P) can be directly obtained from $\Psi_Q(x,y)$ and the corresponding values of $f_a(X_U,W_U)$ and $f_b(X_U,W_U)$ can be uniquely calculated (for convenience, the values of $f_a(X_U,W_U)$ and $f_b(X_U,W_U)$ are denoted as r and w, respectively). X_U and W_U can be obtained by solving Eqs. (8a) and (8b).

$$f_a(X_U, W_U) = r \quad (8a)$$

$$f_b(X_U, W_U) = w \quad (8b)$$

Herein, we adopt a geometric approach to solve Eqs. (9a) and (9b). In this approach, we systematically change the values of X_U and W_U.

Both 1D and 2D spectra are produced according to Eqs. (3), (4) and (5). Then x_A, y_A x_B and y_B are acquired so that the values of $f_a(X_U,W_U)$ and $f_b(X_U,W_U)$ are calculated according to Eq. (9a) and Eq. (9b). via the above procedure, two 2D contour maps for $Z_a = f_a(X_U,W_U)$ and $Z_b = f_b(X_U,\Delta W_U)$ are constructed. Eq. (9a) is a section line (denoted as curve r) at altitude of r the contour map $Z_a = f_a(X_U,W_U)$. Similarly, Eq. (9b) is a section line (denoted as curve w) at altitude of w of the contour map $Z_b = f_b(X_U,W_U)$. If we project curve r and curve w onto the X_U/W_U plane. The coordinates of the cross section of the two projections is just the values of X_U and W_U that we need to know.

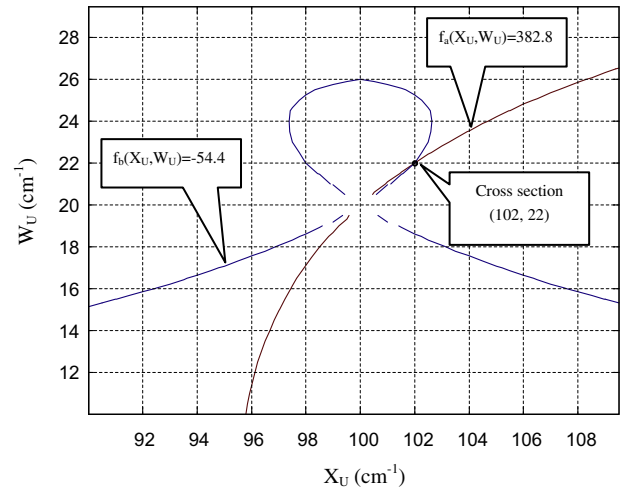


Fig. 3. Projecting section curves ($f_a(X_U,W_U)$ = 382.8 and $f_b(X_U,W_U)$ = −54.4 onto the X_U/W_U plane. The values of X_U and W_U for the specific system can be obtained from the coordinates of the cross section.

We apply this approach to a model chemical system. In order to construct $\Psi_Q(x, y)$, the concentrations of P and Q are selected based on the requirement of the DAOSD approach and listed in Table 1. For a specific model system, the spectral variables for P, Q and V are listed in Table 2. The absorptivity of U (ε_U) is fixed as 1.0 in all the simulation. In the first model system, X_U and W_U are set as 102 cm^{-1} and 22 cm^{-1}, respectively. Both ΔX_P and ΔX_U are only 2 cm^{-1}, while the bandwidth the characteristic peak of P is 20 cm^{-1}. Severe band overlapping occurs in this system. The corresponding 2D asynchronous correlation spectrum was generated and the two independent cross peaks around (X_P,X_P) are (69.5,94.7) and (96.7,121.9), respectively. According to Eq. (8), the value of $f_a(X_U,W_U)$ and $f_b(X_U,W_U)$ are calculated to be

$$f_a(X_U, W_U) = 382.8 \quad (9a)$$

$$f_b(X_U, W_U) = -54.4 \quad (9b)$$

In order to solve Eqs. (9a) and (9b), the values of X_U and W_U are systematically changed. The range of X_U is from 90 cm^{-1} to 110 cm^{-1}

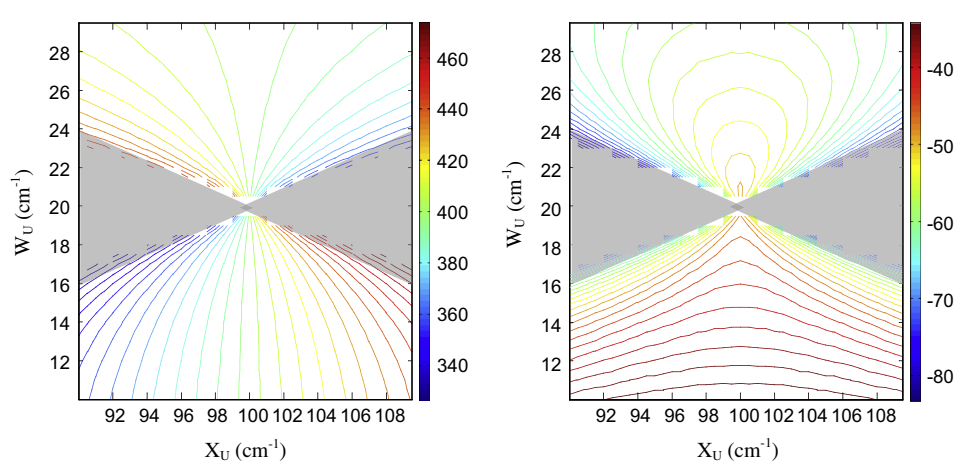
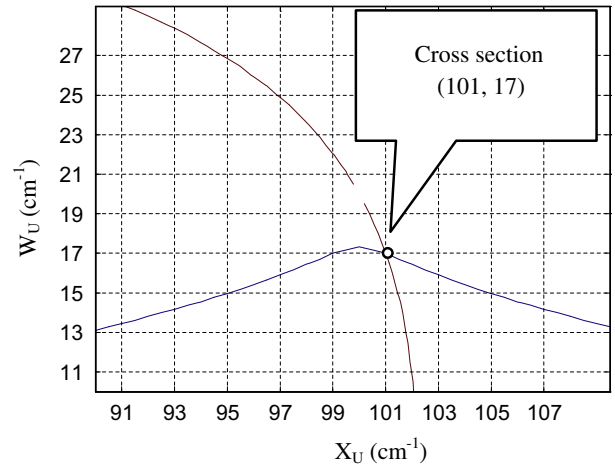
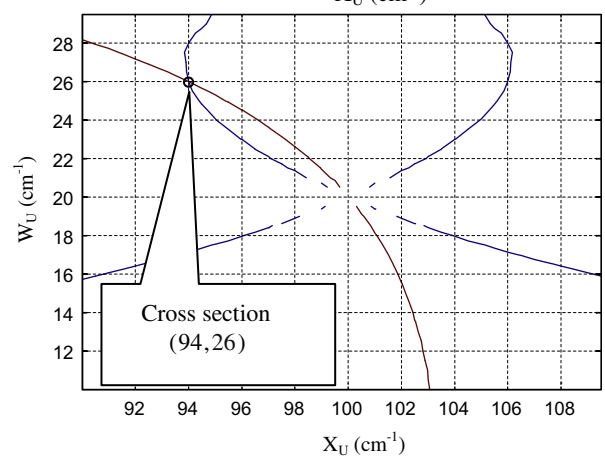
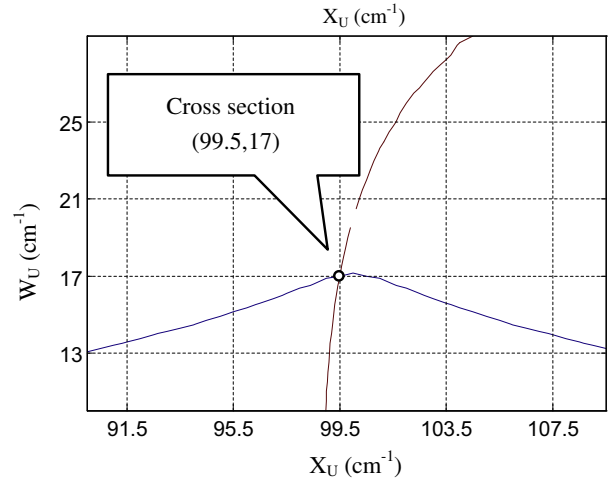


Fig. 2. Contour maps of (a) $f_a(X_U,W_U)$ and (b) $f_b(X_U,W_U)$ for the model chemical system. The dark shade region is not applicable of the algorithm proposed in the paper since only two cross peaks are observed.

Table 3
Calculation results on additional model systems.

Model system	X_U (cm^{-1})	$X_U - X_P$ (cm^{-1})	W_U (cm^{-1})	$W_U - W_P$ (cm^{-1})	Calculation results
1	101	1	17	−3	
2	94	−6	26	6	
3	99.5	−0.5	17	−3	

with a data interval of 0.5 cm^{-1}. The range W_U is from 10 cm^{-1} to 30 cm^{-1} with a data interval of 0.5 cm^{-1}. Two 2D contour maps for $Z_a = f_a(X_U, W_U)$ and $Z_b = f_b(\Delta X_U, \Delta W_U)$ are constructed and shown in Fig. 2. Projection of Eqs. (9a) and (9b) is illustrated in Fig. 3. The coordinates of the cross section of the projections are 102 cm^{-1} and 22 cm^{-1}, respectively. These values are just the same as the X_U and W_U values set for this model system.

To further check whether this approach is reliable or not, we have selected several other model systems whose X_U and W_U values are listed in Table 3. The coordinates of the cross sections are also summarized in Table 3. For each of the model system, X_U and W_U values are reliably reproduced, demonstrating the effectiveness of this approach.

It should be pointed out that the approach described in this paper has some limitation. If ΔX_P is much larger, while the value of ΔW_P is relatively small, only two cross peaks that are anti-symmetric about the diagonal can be observed. Since there are only two independent peak positions available, the approach described in this paper is not applicable to these systems (In Fig. 2a and b, regions marked by dark shade are the region where only two cross peaks are observed). Further work is being performed to explore if it is possible to deduce X_U/W_U in these situation.

In conclusion, we have developed an approach based on the DAOSD method to estimate the variation of peak position and bandwidth of a characteristic peak from a solute involving in intermolecular interaction. The effectiveness of this approach has been validated via computer simulation on a model system. This approach can be used as a novel resolution enhancement method that can differentiate highly overlapping band that are produced by intermolecular interaction.

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