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## Vibrational Dynamics of a Methionine Containing Tripeptide Glycyl-methionyl-glycine

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### ABSTRACT

The mechanism of metal ions binding/coordination with peptides requires a vibrational dynamics study of competing peptides due to the potential antitumor effect of the corresponding metal ions. In the present study, normal mode analysis of a model tripeptide (glycyl-methionyl-glycine) is reported by using the method of Urey Bradley's force field. There are 34 atoms in this tripeptide which gives rise to 96 normal modes of vibrations. For better understanding, these normal frequencies are discussed under three separate headings viz., amide modes, side chain modes and mixed mode. The calculated frequencies are found to be in reasonably good agreement with the reported experimental IR spectra.

**Key words:** Vibrational dynamics, glycyl-methionyl-glycine, normal modes, FT-IR, antitumor drug

### INTRODUCTION

Investigation on coordination and binding of metal ions with proteins and peptides arises due to potential antitumor effect of the corresponding coordination compounds (Reedijk, 1996; Zamble and Lippard, 1995). The study of vibrational dynamics is considered to be an important tool for understanding the mechanism of metal ions coordination with proteins or peptides. Therefore, in the present study the vibrational dynamics of a model tripeptide glycyl-methionyl-glycine (Fig. 1a) has been performed. This investigation will open our understanding for coordination

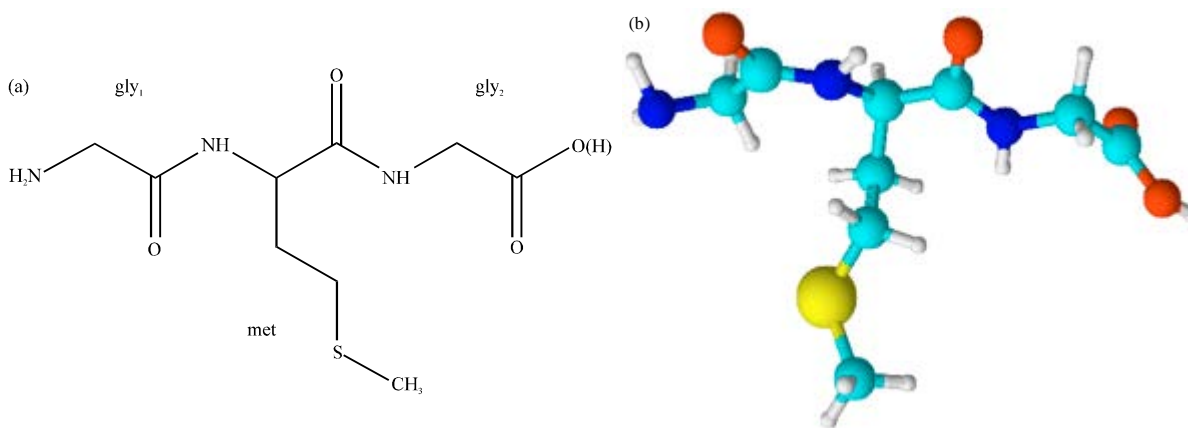


Fig. 1(a-b): (a) Chemical structure of glycyl-methionyl-glycine and (b) Structure of glycyl-methionyl-glycine obtained by molecular modelling (blue: nitrogen, red: oxygen, white: hydrogen, yellow: sulphur, green: carbon)

ability of peptides. Chemically glycyl-methionyl-glycine (H-Gly-Met-Gly-OH) is 2-amino-4-[(2-aminoacetyl)amino]-6-methylsulfanyl-3-oxohexanoic acid having molecular formula  $C_9H_{17}N_3O_4S$  and molecular weight 263.31398 ( $g\ mol^{-1}$ ).

The scientific literatures demonstrated that vibrational dynamics is a potent emerging tool for understanding thermodynamics of macromolecular systems (Taddei *et al.*, 2001). In the thermodynamical study of proteins/peptides, analysis of normal modes is essential to understand the thermodynamical behavior of molecule. In the literatures, several spectroscopic studies of glycine and methionine containing peptides have been reported (Ivanova *et al.*, 2006a). Recently, Ivanova *et al.* (2006b) have reported structural analysis of the tripeptide glycyl-methionyl-glycine. They demonstrated the possibilities of IR-LD spectroscopy for the structural characterization of the amorphous samples which cannot be determined by diffraction methods; and also concluded necessity of a comparative analysis between theoretical and experimental data, especially in case of coordination processes where a conformational distortion is possible (Ivanova *et al.*, 2006a). However, to the best of our knowledge the complete vibrational dynamics of glycyl-methionyl-glycine has not been reported. The other authors also concluded that the normal mode calculations have proved remarkably successful in analyzing vibrational spectra of relatively simple peptides. It has also provided a theoretical basis for understanding structural correlation of complex systems such as proteins and peptides (Bretscher *et al.*, 2001; Srivastava *et al.*, 2000, 2002).

In the continuation of ongoing research work on the vibrational dynamics for numerous polypeptides (Srivastava *et al.*, 1997, 2002; Gupta *et al.*, 1973, 1975, 1997; Srivastava and Gupta, 1974; Burman *et al.*, 1996; Bahuguna *et al.*, 1996; Schweitzer-Stenner, 2006), we reported normal mode calculation and force constant evaluation of a methionine-containing tripeptide glycyl-methionyl-glycine. The present investigation is of topical interest due to the presence of thioether group in the methionine residue of tripeptide. In the present analysis, normal mode analysis was carried out by Wilson's GF matrix method. The IR spectrum of tripeptide (gly-met-gly) used in the present study was reported by Ivanova *et al.* (2006b).

## THEORY

The calculation of normal mode frequencies has been carried out according to the well known Wilson's GF matrix method (Wilson *et al.*, 1980). The force constants have been obtained by least square fitting as described by Srivastava *et al.* (2008). The details of these methods are presented.

**Molecular vibrations of finite molecules:** The molecular dynamics of a finite molecule are considered first. A molecule with N atoms has  $3N-6$  vibrational degrees of freedom (or  $3N-5$  if the molecule is linear). In the Wilson's GF matrix method (Wilson, 1939; Wilson *et al.*, 1955), the concept of 'internal coordinates' is introduced in order to describe the relative motion of various atoms with respect to each other. These internal coordinates are the changes in bond lengths, bond angles, out-of-plane bending and dihedral angles. The advantage of using internal coordinates is that it makes the problem more coherent and even the force constants in terms of these internal coordinates have a more easily visualized physical meaning than others. The force constants can be transferred from one molecule to another if they belong to the same chemical group. In this method, the transformation of Cartesian coordinates to internal coordinates in matrix vector notation is given by:

$$R = BX \tag{1}$$

where, R is the internal coordinate and B is the transformation matrix. Then, the G-matrix or the inverse kinetic energy matrix is defined by the relation given below:

$$G_{kl} = \sum_{i=1}^{3n} \frac{B_k B_l}{m_i} \quad (k, l = 1, \dots, 3n - 6)$$

where  $m_i$  is the mass of the  $i$ th atom.

The kinetic energy is given by:

$$2T = \dot{R} G^{-1} \dot{R} \tag{2}$$

where, R' denotes the transpose of R.

The potential energy is given by the expression:

$$2V = R'FR \tag{3}$$

in which the elements  $F_{kl}$  are the force constants.

The molecular vibrational problem is then represented by the matrix equation:

$$GFL = L\lambda \tag{4}$$

where, the vibrational frequencies are given by  $\lambda = 4\pi^2c^2\nu^2$  and the normal coordinates Q are related to the internal coordinates R by:

$$R = LQ \tag{5}$$

The vibrational dynamics problem thus leads to the secular equation:

$$[GF - \lambda] = 0 \tag{6}$$

that must be solved to obtain the vibrational frequencies ' $\nu$ '.

The eigenvectors L of the dynamical matrix are obtained from the solution of the matrix Eq. 4. The normal coordinates Q are related to the internal displacement coordinates by the linear transformation 5. The extent of vibrational coupling between the various internal displacement coordinates in a given normal mode  $Q_k$  is qualitatively described by the elements of the eigenvector  $L_k$  belonging to the eigenvector  $\lambda_k$ . The fractional Potential Energy Distribution (PED) is useful in making assignments of various frequencies, by analyzing the contributions made from various motions.

In the present study, the Urey-Bradley force field method (Urey and Bradley, 1931) was used to evaluate both bonded and nonbonded interactions as well as internal torsions. The potential energy can be written as:

$$\begin{aligned}
 V = & \sum_{m, j, k} K'_{jk} r_{jk}^m (\Delta r_{jk}^m) + \frac{1}{2} K_{jk} (\Delta r_{jk}^m)^2 + \sum_{m, i, j, k} H'_{ijk} r_{ij}^m r_{jk}^m (\Delta \alpha_{ijk}^m) \\
 & + \frac{1}{2} [H_{ijk} r_{ij}^m r_{jk}^m (\Delta \alpha_{ijk}^m)^2] + \sum_{m, i, j, k} F'_{jk} q_{ik}^m (\Delta q_{ik}^m) + \frac{1}{2} [F_{ik} (\Delta q_{ik}^m)^2] \\
 & + \sum_j k_j^r (\Delta \tau_j)^2 + \sum_j k_j^w (\Delta \omega_j)^2
 \end{aligned}$$

where, the symbols have their usual meaning (Wilson *et al.*, 1955). The primed quantities are introduced as internal torsions. Nonbonded interactions involve attraction and repulsion of atoms due to the overlap of their electron orbitals. The effects are usually expressed by 6-exp or 6-12 type potentials. The tension terms are assumed to be 1/10 of the non-bonded interactions.

**Force constants evaluation:** The force constants have been obtained by least square fitting. In order to obtain the best fit with the observed frequencies the following procedure was adopted. Initially force constants for the backbone were transferred from the other polypeptides having similar conformation. Thus, starting with the approximate F matrix,  $F_0$  and the observed frequencies  $\lambda_{obs}$  (related through a constant), one can solve the secular matrix equation:

$$GF_0L_0 = L_0\lambda_0 \quad (7)$$

Let  $\Delta\lambda_i = \lambda_{i_{obs}} - \lambda_{i_0}$  in the above equation. It can be shown that in the first order approximation:

$$\Delta\lambda = J\Delta F \quad (8)$$

where, J is computed from  $L_0$ . We wish to compute the corrections to  $F_0$  so that the errors  $\Delta\lambda$  are minimized. The theory of least squares was used to calculate:

$$J'P\Delta\lambda = (J'PJ)\Delta F \quad (9)$$

The solution to this equation is obtained by inverting  $(J'PJ)$  to give:

$$\Delta F = (J'PJ)^{-1} J'P\Delta\lambda \quad (10)$$

If the number of frequencies is greater than the number of F matrix elements, the matrix  $J'PJ$  should be non-singular and we obtain the corrections  $\Delta F$  which will minimize the sum of the weighed squares of the residuals. If the corrections are fairly large, the linear relation between force constant and frequency term in the matrix equation 7 breaks down. In such a situation, further refinement using higher order terms in the Taylor's series expansion of  $\Delta\lambda_i$  is needed. This procedure has been developed by King *et al.* (1957).

**Molecular modelling and experimental model:** The software used for molecular modelling and energy minimization of glycyle-methionyl-glycine was ACD Lab. In order to check the stereo-chemical quality of structure and to obtain Ramachandran plots, Procheck 3.4 for Windows NT was used. This is a 32 bit Windows version of the Procheck program proposed by Laskowski *et al.* (1993). Basically it works as follows. In order to obtain probable conformations characterized by the dihedral angles  $\phi$ ,  $\psi$ ,  $\omega$  (in the main chain) and  $\chi_1$ ,  $\chi_2$ ,  $\chi_3$ ,..... (in the side

chain) corresponding to global energy minimization, the method of Ramachandran *et al.* (1963) was used. It consists of calculating the inter-atomic distances for all the atoms and all ranges of the dihedral angles which are of interest. The Cartesian coordinates were evaluated for the conformations corresponding to the state of global energy minimization for the tripeptide.

In this study, we used 3500-500  $\text{cm}^{-1}$  solid-state IR-spectra of glycyl-methionyl-glycine recorded on a Bomem Michelson 100 FT-IR Spectrometer (resolution  $\pm 2 \text{ cm}^{-1}$ , 150 scans) by Ivanova *et al.* (2006a) structure of glycyl-methionyl-glycine obtained by molecular modelling is given in Fig. 1b.

## RESULTS AND DISCUSSION

Glycyl-methionyl-glycine has 34 atoms which give rise to 96 normal modes of vibrations. Initially, the force constants for the backbone and the side chain modes were transferred from other glycine and methionine containing peptides (Kumar, 1997; Kumar *et al.*, 2007) and then modified in order to obtain the "best fit" with the spectroscopic data. The calculated force constants (dynes/cm) and internal coordinates for gly-met-gly are given in Table 1. The assignments of modes were made on the basis of potential energy distribution, line shape and intensity, derivative spectra and the presence/absence of modes present in similar environment in other molecules. Glycyl-methionyl-glycine has two peptide groups, belonging to methionine and glycine residues which give rise to characteristic amide modes. For the sake of simplicity, the assignments of the modes are discussed under three separate headings such as amide (back bone) modes, side modes and mixed modes. All these modes are given in Table 2-4. The calculated frequencies are compared with the observed ones.

Table 1: Internal coordinates and force constants (dynes/cm) of gly-met-gly

Internal coordinates	Force constants
$\nu(\text{N-H})$	5.300
$\nu(\text{N-C}\alpha)$	2.600
$\nu(\text{C}\alpha\text{-H})$	4.950
$\nu(\text{C}\alpha\text{-C})$	2.100
$\nu(\text{C}=\text{O})$	10.150
$\nu(\text{C-N})$	5.800
$\nu(\text{C}\alpha\text{-C}\beta)$	3.300
$\nu(\text{C}\beta\text{-H})$	4.850
$\nu(\text{C}\beta\text{-C}\gamma)$	2.900
$\nu(\text{C}\gamma\text{-H})$	4.900
$\nu(\text{C}\gamma\text{-S})$	3.900
$\nu(\text{C-S})$	2.650
$\nu(\text{C-H})$	4.230
$\nu(\text{C-O})$	3.600
$\nu(\text{O-H})$	5.950
$\phi(\text{H-N-H})$	0.470 (0.40)
$\phi(\text{H-N-C}\alpha)$	0.420 (0.60)
$\phi(\text{N-C}\alpha\text{-H})$	0.430 (0.60)
$\phi(\text{N-C}\alpha\text{-C})$	0.450 (0.50)
$\phi(\text{H-C}\alpha\text{-H})$	0.130 (0.18)
$\phi(\text{H-C}\alpha\text{-C})$	0.410 (0.18)
$\phi(\text{C}\alpha\text{-C}=\text{O})$	0.200 (0.60)
$\phi(\text{C}\alpha\text{-C-N})$	0.210 (0.50)

Table 1: Continue

Internal coordinates	Force constants
$\varphi(\text{O} = \text{C}-\text{N})$	0.550 (0.90)
$\varphi(\text{C}-\text{N}-\text{H})$	0.220 (0.60)
$\varphi(\text{C}-\text{N}-\text{C}\alpha)$	0.530 (0.35)
$\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$	0.420 (0.50)
$\varphi(\text{H}-\text{C}\alpha-\text{C}\beta)$	0.260 (0.20)
$\varphi(\text{C}\beta-\text{C}\alpha-\text{C})$	0.520 (0.18)
$\varphi(\text{C}\alpha-\text{C}\beta-\text{H})$	0.450 (0.20)
$\varphi(\text{C}\alpha-\text{C}\beta-\text{C}\gamma)$	0.520 (0.18)
$\varphi(\text{H}-\text{C}\beta-\text{H})$	0.345 (0.24)
$\varphi(\text{H}-\text{C}\beta-\text{H})$	0.420 (0.20)
$\varphi(\text{C}\beta-\text{C}\gamma-\text{H})$	0.447 (0.25)
$\varphi(\text{C}\beta-\text{C}\gamma-\text{S})$	0.450 (0.22)
$\varphi(\text{H}-\text{C}\gamma-\text{S})$	0.461 (0.111)
$\varphi(\text{H}-\text{C}\gamma-\text{H})$	0.330 (0.24)
$\varphi(\text{C}\gamma-\text{S}-\text{C})$	0.300 (0.25)
$\varphi(\text{S}-\text{C}-\text{H})$	0.380 (0.111)
$\varphi(\text{H}-\text{C}-\text{H})$	0.405 (0.30)
$\varphi(\text{C}\alpha-\text{C}-\text{O})$	0.250 (0.40)
$\varphi(\text{C}-\text{O}-\text{H})$	0.450 (0.25)
$\omega(\text{N}-\text{H})$	0.095
$\omega(\text{C}\alpha-\text{H})$	0.080
$\omega(\text{C} = \text{O})$	0.535
$\omega(\text{C}\beta-\text{H})$	0.100
$\omega(\text{C}\gamma-\text{H})$	0.170
$\omega(\text{C}-\text{H})$	0.050
$\tau(\text{C}\alpha-\text{N})$	0.005
$\tau(\text{C}\alpha-\text{C})$	0.100
$\tau(\text{C}-\text{N})$	0.010
$\tau(\text{C}\alpha-\text{C}\beta)$	0.100
$\tau(\text{C}\beta-\text{C}\gamma)$	0.050
$\tau(\text{C}\gamma-\text{S})$	0.043
$\tau(\text{C}-\text{S})$	0.043
$\tau(\text{C}-\text{O})$	0.100

v,  $\varphi$ ,  $\omega$ ,  $\tau$  represent stretch, angle bends, wags and torsions, respectively. Non-bonded force constants are given in parenthesis

**Amide modes:** The tripeptide glycyl-methionyl-glycine consists of amide groups joined together by  $\text{C}\alpha$  atoms. The modes involving the motion of the amide group  $\text{N}-\text{C}\alpha$ ,  $\text{C}-\text{C}\alpha$  stretches,  $\text{C}-\text{C}\alpha-\text{N}$  bending and their mixtures are regarded as skeletal or backbone modes. Pure backbone modes are given in Table 2. Normally, in a regular peptide structure, the interaction between the side chain and the main chain is weak. However, when the structure is irregular there is every likelihood of a strong interaction between the atoms/groups of the side chain and main chain atoms. This will lead to strong mixing and shifted appearances of modes which would have, otherwise, appeared single in a regular structure. In the spectra of proteins and peptides, there are number of bands which are characteristics of the peptide bond. The positions of these bands are sensitive to the peptide conformation. Thus, IR spectroscopy, in combination with normal coordinate analysis, has been shown to be a very useful tool for structural investigations. This is generally done in terms of amide band positions.

Table 2: Comparison of calculated and observed frequencies for pure back bone modes of glycyl-methionyl-glycine

Calculation	Observation	Assignments
3304	3300	$\nu(\text{O-H})$ (100)
3282	3285	$\nu(\text{N-H})$ (100) AMIDE A
3270		$\nu(\text{N-H})$ (100)
3262		$\nu(\text{N-H})$ (101)
3182		$\nu(\text{N-H})$ (103)
1729	1735	$\nu(\text{C}=\text{O})$ (83)+ $\nu(\text{C-N})$ (17) AMIDE I
1726	1735	$\nu(\text{C}=\text{O})$ (82)+ $\nu(\text{C-N})$ (18) AMIDE I
1674	1685	$\nu(\text{C}=\text{O})$ (96)
1670	1668	$\varphi(\text{H-N-H})$ (82)+ $\varphi(\text{H-N-C}\alpha)$ (9)+ $\omega(\text{N-H})$ (9) AMIDE II
1608	1602	$\varphi(\text{N-C}\alpha\text{-H})$ (17)+ $\varphi(\text{H-C}\alpha\text{-H})$ (68)
1520	1517	$\nu(\text{N-C}\alpha)$ (5)+ $\nu(\text{C-N})$ (23)+ $\varphi(\text{H-N-C}\alpha)$ (50)+ $\varphi(\text{C-N-H})$ (29)
1516	1517	$\nu(\text{C}=\text{O})$ (8)+ $\varphi(\text{H-N-C}\alpha)$ (60)+ $\varphi(\text{C-N-H})$ (30)
1358	1357	$\nu(\text{N-C}\alpha)$ (7)+ $\nu(\text{C-N})$ (20)+ $\varphi(\text{H-N-C}\alpha)$ (12)+ $\varphi(\text{N-C}\alpha\text{-H})$ (41)+ $\varphi(\text{H-C}\alpha\text{-C})$ (11)
1324	1321	$\nu(\text{C}\alpha\text{-C})$ (20)+ $\nu(\text{C}=\text{O})$ (8)+ $\nu(\text{C-N})$ (40)+ $\varphi(\text{H-N-C}\alpha)$ (10)+ $\varphi(\text{N-C}\alpha\text{-H})$ (11)+ $\varphi(\text{O}=\text{C-N})$ (6) AMIDE III
1319	1321	$\nu(\text{C}\alpha\text{-C})$ (10)+ $\varphi(\text{N-C}\alpha\text{-H})$ (43)+ $\varphi(\text{H-C}\alpha\text{-H})$ (6)+ $\varphi(\text{H-C}\alpha\text{-C})$ (44)
1303	1302	$\varphi(\text{H-N-C}\alpha)$ (44)+ $\varphi(\text{N-C}\alpha\text{-H})$ (44)+ $\omega(\text{N-H})$ (7)
1252	1250	$\varphi(\text{N-C}\alpha\text{-H})$ (78)+ $\varphi(\text{H-C}\alpha\text{-C})$ (15)
1230	1224	$\varphi(\text{H-N-C}\alpha)$ (66)+ $\varphi(\text{N-C}\alpha\text{-H})$ (16)+ $\varphi(\text{H-C}\alpha\text{-H})$ (8)
1178	1178	$\varphi(\text{H-N-C}\alpha)$ (36)+ $\varphi(\text{N-C}\alpha\text{-H})$ (37)+ $\varphi(\text{H-C}\alpha\text{-C})$ (20)+ $\omega(\text{N-H})$ (9)
1079	1071	$\nu(\text{C}\alpha\text{-C})$ (13)+ $\varphi(\text{O}=\text{C-N})$ (9)+ $\varphi(\text{C-O-H})$ (65)
1039	1041	$\nu(\text{N-C}\alpha)$ (69)+ $\varphi(\text{N-C}\alpha\text{-C})$ (8)+ $\omega(\text{C}=\text{O})$ (7)
1017	1017	$\nu(\text{N-C}\alpha)$ (92)
734	732	$\nu(\text{N-C}\alpha)$ (6)+ $\nu(\text{C}\alpha\text{-C})$ (27)+ $\varphi(\text{N-C}\alpha\text{-C})$ (8)+ $\varphi(\text{H-C}\alpha\text{-C})$ (7)+ $\omega(\text{N-H})$ (7)+ $\omega(\text{C}=\text{O})$ (23) AMIDE V
718	714	$\nu(\text{C}\alpha\text{-C})$ (11)+ $\nu(\text{C-O})$ (15)+ $\varphi(\text{H-C}\alpha\text{-C})$ (8)+ $\omega(\text{N-H})$ (10)+ $\omega(\text{C}=\text{O})$ (24)
521	519	$\varphi(\text{N-C}\alpha\text{-C})$ (18)+ $\varphi(\text{C}\alpha\text{-C}=\text{O})$ (19)+ $\varphi(\text{O}=\text{C-N})$ (30)+ $\omega(\text{N-H})$ (7)
514	519	$\varphi(\text{N-C}\alpha\text{-C})$ (9)+ $\varphi(\text{C}\alpha\text{-C}=\text{O})$ (12)+ $\varphi(\text{O}=\text{C-N})$ (40)+ $\tau(\text{C-O})$ (9)
484	500	$\omega(\text{N-H})$ (57)+ $\omega(\text{C}=\text{O})$ (10)+ $\tau(\text{C-N})$ (10)
456		$\varphi(\text{C}\alpha\text{-C}=\text{O})$ (9)+ $\varphi(\text{O}=\text{C-N})$ (8)+ $\omega(\text{N-H})$ (5)+ $\omega(\text{C}=\text{O})$ (10)+ $\tau(\text{C-O})$ (36)
447		$\nu(\text{C}\alpha\text{-C})$ (7)+ $\varphi(\text{C}\alpha\text{-C}=\text{O})$ (9)+ $\varphi(\text{C}\alpha\text{-C-N})$ (9)+ $\varphi(\text{O}=\text{C-N})$ (8)+ $\varphi(\text{C-N-C}\alpha)$ (6)+ $\omega(\text{C}=\text{O})$ (8)+ $\tau(\text{C-O})$ (18)
362		$\varphi(\text{N-C}\alpha\text{-C})$ (7)+ $\varphi(\text{C}\alpha\text{-C}=\text{O})$ (23)+ $\varphi(\text{O}=\text{C-N})$ (7)+ $\varphi(\text{C}\alpha\text{-C-O})$ (28)
268		$\varphi(\text{N-C}\alpha\text{-C})$ (41)+ $\varphi(\text{C}\alpha\text{-C}=\text{O})$ (8)+ $\varphi(\text{O}=\text{C-N})$ (12)+ $\varphi(\text{C-N-C}\alpha)$ (7)
102		$\varphi(\text{N-C}\alpha\text{-C})$ (6)+ $\varphi(\text{C-N-C}\alpha)$ (6)+ $\omega(\text{C}=\text{O})$ (5)+ $\tau(\text{C}\alpha\text{-C})$ (53)+ $\tau(\text{C-N})$ (7)
92		$\omega(\text{C}=\text{O})$ (7)+ $\tau(\text{C}\alpha\text{-C})$ (61)
67		$\tau(\text{C}\alpha\text{-N})$ (83)+ $\tau(\text{C}\alpha\text{-C})$ (8)
48		$\varphi(\text{N-C}\alpha\text{-C})$ (7)+ $\varphi(\text{C-N-C}\alpha)$ (6)+ $\tau(\text{C}\alpha\text{-N})$ (13) + $\tau(\text{C}\alpha\text{-C})$ (45)
9		$\tau(\text{C}\alpha\text{-N})$ (32)+ $\tau(\text{C-N})$ (54)
7		$\tau(\text{C}\alpha\text{-N})$ (82)+ $\tau(\text{C-N})$ (6)

$\nu$ ,  $\varphi$ ,  $\omega$ ,  $\tau$  represent stretch, angle bends, wags and torsions, respectively

In this tripeptide, amide A band (due to N-H stretch) is calculated at  $3282\text{ cm}^{-1}$ . This mode is assigned to observed value at  $3282\text{ cm}^{-1}$ . Another peptide L-prolyl-glycyl-glycine also showed amide A in the same range (Kumar *et al.*, 2007). Amide A mode is not sensitive to conformation but highly depends on the strength of the hydrogen bond. Amide I mode (due to C = O and C-N stretches) which is well known for peptide conformation (Schweitzer-Stenner, 2006), is calculated at  $1729$  and  $1726\text{ cm}^{-1}$  and assigned to IR absorption band at  $1735\text{ cm}^{-1}$ . The frequency calculated at  $1670\text{ cm}^{-1}$  is of amide II and assigned to IR absorption band at  $1668\text{ cm}^{-1}$ . These modes have mixed



Table 3: Comparison of calculated and observed frequencies for side chain modes of glycyl-methionyl-glycine

Calculation	Observation	Assignments
3151	3160	$\nu(\text{C}\alpha\text{-H})$ (102)
3150	3160	$\nu(\text{C}\alpha\text{-H})$ (103)
3144	3160	$\nu(\text{C}\alpha\text{-H})$ (100)
3143		$\nu(\text{C}\alpha\text{-H})$ (98)
3142		$\nu(\text{C}\alpha\text{-H})$ (97)
3085	3072	$\nu(\text{C}\beta\text{-H})$ ( 58)+ $\nu(\text{C}\gamma\text{-H})$ (40)
3094		$\nu(\text{C}\beta\text{-H})$ ( 40)+ $\nu(\text{C}\gamma\text{-H})$ (58)
3076	3072	$\nu(\text{C}\gamma\text{-H})$ ( 99)
3071	3071	$\nu(\text{C}\beta\text{-H})$ ( 99)
2959		$\nu(\text{C-H})$ ( 92)
2878	2875	$\nu(\text{C-H})$ (105)
2877	2875	$\nu(\text{C-H})$ (105)
1489	1482	$\phi(\text{H-C-H})$ (91)+ $\omega(\text{C-H})$ (6)
1479	1482	$\phi(\text{H-C-H})$ (91)+ $\omega(\text{C-H})$ (5)
1450	1446	$\phi(\text{H-C}\beta\text{-H})$ (17)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (9)+ $\phi(\text{H-C}\gamma\text{-S})$ (6)+ $\phi(\text{H-C}\gamma\text{-H})$ (47)+ $\omega(\text{C}\gamma\text{-H})$ (9)
1384	1374	$\nu(\text{C-S})$ (6)+ $\phi(\text{S-C-H})$ (39)+ $\phi(\text{H-C-H})$ (51)+ $\omega(\text{C-H})$ (9)
1355	1357	$\nu(\text{C}\alpha\text{-C}\beta)$ (17)+ $\nu(\text{C}\beta\text{-C}\gamma)$ (19)+ $\nu(\text{C}\gamma\text{-S})$ (5)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (22)+ $\phi(\text{H-C}\beta\text{-H})$ (29)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (11)+ $\phi(\text{H-C}\gamma\text{-S})$ (9)
1264	1268	$\nu(\text{C}\gamma\text{-S})$ (9)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (12)+ $\phi(\text{H-C}\beta\text{-H})$ (14)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (33)+ $\phi(\text{H-C}\gamma\text{-S})$ (26)
878	893	$\nu(\text{C}\alpha\text{-C}\beta)$ (16)+ $\nu(\text{C}\beta\text{-C}\gamma)$ (9)+ $\nu(\text{C}\gamma\text{-S})$ (18)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (7)+ $\phi(\text{S-C-H})$ (7)
41		$\tau(\text{C}\alpha\text{-C}\beta)$ (14)+ $\tau(\text{C}\beta\text{-C}\gamma)$ (30)+ $\tau(\text{C}\gamma\text{-S})$ (44)

$\nu$ ,  $\phi$ ,  $\omega$ ,  $\tau$  represent stretch, angle bends, wags and torsions, respectively

Table 4: Comparison of calculated and observed frequencies for mix modes of glycyl-methionyl-glycine

Calculation	Observation	Assignments
1408	1410	$\nu(\text{C-N})$ (8)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (5)+ $\phi(\text{H-C}\beta\text{-H})$ (40)+ $\phi(\text{H-C}\gamma\text{-H})$ (15)
1400	1410	$\nu(\text{C}\alpha\text{-C})$ (17)+ $\nu(\text{C-N})$ (31)+ $\phi(\text{H-N-C}\alpha)$ (6)+ $\phi(\text{N-C}\alpha\text{-H})$ (16)+ $\phi(\text{H-C}\alpha\text{-C})$ (6)+ $\phi(\text{H-C}\beta\text{-H})$ (11)
1288	1285	$\nu(\text{C-N})$ (16)+ $\phi(\text{N-C}\alpha\text{-H})$ (53)+ $\phi(\text{H-C}\alpha\text{-C})$ (7)+ $\phi(\text{H-C}\alpha\text{-C}\beta)$ (6)
1194	1196	$\nu(\text{C}\alpha\text{-C})$ (5)+ $\nu(\text{C}\alpha\text{-C}\beta)$ (16)+ $\phi(\text{H-C}\alpha\text{-C})$ (20)+ $\phi(\text{H-C}\alpha\text{-C}\beta)$ (17)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (16)+ $\phi(\text{H-C}\beta\text{-H})$ (10)
1161	1160	$\nu(\text{C}\alpha\text{-C}\beta)$ (5)+ $\phi(\text{H-C}\alpha\text{-C})$ (8)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (12)+ $\phi(\text{H-C}\beta\text{-H})$ (37)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (19)
1146	1141	$\nu(\text{N-C}\alpha)$ (11)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (21)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (37)+ $\phi(\text{H-C}\gamma\text{-S})$ (9)
1098	1089	$\nu(\text{N-C}\alpha)$ (9)+ $\nu(\text{C}\alpha\text{-C})$ (5)+ $\phi(\text{H-N-C}\alpha)$ (7)+ $\phi(\text{H-C}\alpha\text{-H})$ (34)+ $\phi(\text{H-C}\alpha\text{-C})$ (34)+ $\omega(\text{C}\alpha\text{-H})$ (6)
1073	1071	$\nu(\text{N-C}\alpha)$ (33)+ $\phi(\text{H-C}\alpha\text{-C})$ (9)+ $\phi(\text{H-C}\beta\text{-H})$ (6)+ $\phi(\text{C}\beta\text{-C}\gamma\text{-H})$ (7)+ $\phi(\text{H-C}\gamma\text{-S})$ (16)
1013	1017	$\phi(\text{H-C}\alpha\text{-C})$ (7)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (13)+ $\phi(\text{H-C}\gamma\text{-S})$ (38)+ $\omega(\text{C}\gamma\text{-H})$ (13)
986	979	$\nu(\text{C}\alpha\text{-C})$ (17)+ $\nu(\text{C-O})$ (24)+ $\phi(\text{H-C}\alpha\text{-C})$ (26)+ $\phi(\text{C}\alpha\text{-C}=\text{O})$ (5)+ $\phi(\text{C-O-H})$ (20)+ $\omega(\text{C}\alpha\text{-H})$ (7)
979	964	$\nu(\text{N-C}\alpha)$ (5)+ $\nu(\text{C}\alpha\text{-C}\beta)$ (6)+ $\nu(\text{C}\beta\text{-C}\gamma)$ (36)+ $\phi(\text{H-C}\alpha\text{-C})$ (6)+ $\phi(\text{H-C}\beta\text{-H})$ (7)
965	964	$\nu(\text{C}\beta\text{-C}\gamma)$ (7)+ $\phi(\text{N-C}\alpha\text{-H})$ (9)+ $\phi(\text{H-C}\alpha\text{-C})$ (42)+ $\omega(\text{C}\alpha\text{-H})$ (12)+ $\omega(\text{C}=\text{O})$ (15)
936	946	$\nu(\text{C}\alpha\text{-C})$ (15)+ $\nu(\text{C}\alpha\text{-C}\beta)$ (6)+ $\nu(\text{C}\beta\text{-C}\gamma)$ (6)+ $\phi(\text{H-C}\alpha\text{-C})$ (9)+ $\phi(\text{H-C}\beta\text{-H})$ (11)+ $\phi(\text{H-C}\gamma\text{-S})$ (8)+ $\omega(\text{C}\gamma\text{-H})$ (7)
902	905	$\nu(\text{C}\alpha\text{-C})$ (22)+ $\nu(\text{C-O})$ (21)+ $\phi(\text{H-C}\alpha\text{-C})$ (31)+ $\phi(\text{O}=\text{C-N})$ (6)+ $\phi(\text{C-O-H})$ (7)+ $\omega(\text{C}\alpha\text{-H})$ (8)
866	875	$\phi(\text{S-C-H})$ (81)+ $\omega(\text{C-H})$ (10)
858	857	$\nu(\text{C}\alpha\text{-C})$ (21)+ $\nu(\text{C}\gamma\text{-S})$ (9)+ $\phi(\text{O}=\text{C-N})$ (6)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (7)+ $\phi(\text{S-C-H})$ (8)
849	857	$\nu(\text{C}\alpha\text{-C})$ (7)+ $\nu(\text{C}\gamma\text{-S})$ (23)+ $\phi(\text{C}\alpha\text{-C}\beta\text{-H})$ (6)+ $\phi(\text{H-C}\beta\text{-H})$ (7)+ $\phi(\text{S-C-H})$ (24)+ $\omega(\text{C}\beta\text{-H})$ (5)
807	811	$\nu(\text{C}\alpha\text{-C})$ (8)+ $\nu(\text{C}\gamma\text{-S})$ (11)+ $\phi(\text{S-C-H})$ (46)+ $\omega(\text{C}=\text{O})$ (11)
796	788	$\nu(\text{C}\alpha\text{-C})$ (10)+ $\nu(\text{C}\gamma\text{-S})$ (6)+ $\phi(\text{S-C-H})$ (11)+ $\omega(\text{C}=\text{O})$ (30)+ $\tau(\text{C-O})$ (12)
783	788	$\nu(\text{C}\alpha\text{-C})$ (15)+ $\nu(\text{C}\gamma\text{-S})$ (8)+ $\phi(\text{S-C-H})$ (6)+ $\omega(\text{C}=\text{O})$ (33)
702	704	$\nu(\text{C-S})$ (74)+ $\omega(\text{C}=\text{O})$ (7)
698	678	$\nu(\text{C}\alpha\text{-C})$ (18)+ $\nu(\text{C-S})$ (18)+ $\nu(\text{C-O})$ (16)+ $\omega(\text{C}=\text{O})$ (19)
623	613	$\nu(\text{N-C}\alpha)$ (7)+ $\nu(\text{C}\alpha\text{-C})$ (5)+ $\phi(\text{N-C}\alpha\text{-C})$ (5)+ $\phi(\text{O}=\text{C-N})$ (18)+ $\phi(\text{C-N-C}\alpha)$ (12)+ $\phi(\text{N-C}\alpha\text{-C}\beta)$ (8)+ $\omega(\text{C}=\text{O})$ (5)

Table 4: Continue

Calculation	Observation	Assignments
550	546	$\varphi(\text{O} = \text{C}-\text{N})$ (10)+ $\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (8)+ $\omega(\text{N}-\text{H})$ (25)+ $\omega(\text{C} = \text{O})$ (14)
436		$\varphi(\text{C}\alpha-\text{C}-\text{N})$ (5)+ $\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (6)+ $\varphi(\text{C}\alpha-\text{C}\beta-\text{C}\gamma)$ (7)+ $\omega(\text{N}-\text{H})$ (27)+ $\omega(\text{C} = \text{O})$ (10)+ $\tau(\text{C}-\text{O})$ (6)
316		$\nu(\text{N}-\text{C}\alpha)$ (5)+ $\varphi(\text{N}-\text{C}\alpha-\text{C})$ (6)+ $\varphi(\text{C}\alpha-\text{C} = \text{O})$ (12)+ $\varphi(\text{C}\alpha-\text{C}-\text{N})$ (6)+ $\varphi(\text{O} = \text{C}-\text{N})$ (14)+ $\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (12)+ $\varphi(\text{C}\beta-\text{C}\alpha-\text{C})$ (11)+ $\varphi(\text{C}\alpha-\text{C}-\text{O})$ (10)
257		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (16)+ $\varphi(\text{C}\alpha-\text{C} = \text{O})$ (9)+ $\varphi(\text{C}\alpha-\text{C}-\text{N})$ (7)+ $\varphi(\text{C}\beta-\text{C}\gamma-\text{S})$ (23)+ $\varphi(\text{C}\gamma-\text{S}-\text{C})$ (9)
243		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (8)+ $\varphi(\text{C}\alpha-\text{C} = \text{O})$ (6)+ $\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (14)+ $\varphi(\text{C}\beta-\text{C}\gamma-\text{S})$ (8)+ $\varphi(\text{C}\gamma-\text{S}-\text{C})$ (31)
230		$\nu(\text{C}\alpha-\text{C})$ (5)+ $\varphi(\text{N}-\text{C}\alpha-\text{C})$ (6)+ $\varphi(\text{C}\alpha-\text{C} = \text{O})$ (14)+ $\varphi(\text{C}\alpha-\text{C}-\text{N})$ (6)+ $\varphi(\text{O} = \text{C}-\text{N})$ (5)+ $\varphi(\text{C}-\text{N}-\text{C}\alpha)$ (14)+ $\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (5)+ $\varphi(\text{C}\gamma-\text{S}-\text{C})$ (17)
184		$\nu(\text{C}\alpha-\text{C})$ (7)+ $\varphi(\text{C}-\text{N}-\text{C}\alpha)$ (8)+ $\varphi(\text{C}\beta-\text{C}\alpha-\text{C})$ (12)+ $\varphi(\text{C}\beta-\text{C}\gamma-\text{S})$ (15)+ $\varphi(\text{C}\gamma-\text{S}-\text{C})$ (8)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (6)
157		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (37)+ $\tau(\text{C}\alpha-\text{C})$ (6)+ $\tau(\text{C}-\text{S})$ (21)
152		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (9)+ $\tau(\text{C}-\text{S})$ (70)
134		$\varphi(\text{N}-\text{C}\alpha-\text{C}\beta)$ (5)+ $\varphi(\text{C}\alpha-\text{C}\beta-\text{C}\gamma)$ (12)+ $\varphi(\text{C}\beta-\text{C}\gamma-\text{S})$ (11)+ $\varphi(\text{C}\gamma-\text{S}-\text{C})$ (23)+ $\tau(\text{C}\alpha-\text{C})$ (9)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (10)
124		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (8)+ $\varphi(\text{C}\alpha-\text{C} = \text{O})$ (8)+ $\varphi(\text{C}\alpha-\text{C}-\text{N})$ (17)+ $\varphi(\text{O} = \text{C}-\text{N})$ (5)+ $\varphi(\text{C}-\text{N}-\text{C}\alpha)$ (21)+ $\tau(\text{C}\alpha-\text{C})$ (6)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (8)+ $\tau(\text{C}\gamma-\text{S})$ (60)
72		$\varphi(\text{N}-\text{C}\alpha-\text{C})$ (8)+ $\varphi(\text{C}\alpha-\text{C}-\text{N})$ (5)+ $\varphi(\text{C}-\text{N}-\text{C}\alpha)$ (7)+ $\varphi(\text{C}\alpha-\text{C}\beta-\text{C}\gamma)$ (7)+ $\tau(\text{C}\alpha-\text{N})$ (14)+ $\tau(\text{C}\alpha-\text{C})$ (26)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (7)
63		$\varphi(\text{C}\alpha-\text{C}\beta-\text{C}\gamma)$ (5)+ $\tau(\text{C}\alpha-\text{C})$ (14)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (8)+ $\tau(\text{C}\beta-\text{C}\gamma)$ (15)+ $\tau(\text{C}\gamma-\text{S})$ (28)
30		$\varphi(\text{C}\alpha-\text{C}-\text{N})$ (7)+ $\varphi(\text{C}-\text{N}-\text{C}\alpha)$ (5)+ $\alpha(\text{C}\beta-\text{C}\alpha-\text{C})$ (9)+ $\tau(\text{C}\alpha-\text{N})$ (8)+ $\tau(\text{C}-\text{N})$ (13)+ $\tau(\text{C}\alpha-\text{C}\beta)$ (13)+ $\tau(\text{C}\beta-\text{C}\gamma)$ (16)

$\nu$ ,  $\varphi$ ,  $\omega$ ,  $\tau$  represent stretch, angle bends, wags and torsions, respectively

contributions from both peptide units. Amide III due to C-N stretch and N-H in plane deformation is calculated at  $1324 \text{ cm}^{-1}$  and assigned to the observed peak in IR spectra at  $1321 \text{ cm}^{-1}$ . Amide IV is calculated at  $734 \text{ cm}^{-1}$  and assigned to observed value at  $732 \text{ cm}^{-1}$ .

**Side chain modes:** The conformation insensitive  $\text{CH}_2$  scissoring mode in the side chain, calculated at  $1479$  and  $1489 \text{ cm}^{-1}$ , is fitted to the observed band at  $1482 \text{ cm}^{-1}$ . They have been observed at nearly the same value, at  $1460 \text{ cm}^{-1}$  in poly(L-isoleucine) also (LaVerne *et al.*, 2010). The theoretically calculated frequencies at  $878$  and  $1384 \text{ cm}^{-1}$  represents  $\nu(\text{C}\gamma-\text{S})$  and  $\varphi(\text{S}-\text{C}-\text{H})$  bond, respectively; and belong to the S-CH<sub>3</sub> group of methionine residue. These calculated frequencies ( $878$  and  $1384 \text{ cm}^{-1}$ ) are assigned to experimentally obtained IR absorption band at  $893$  and  $1374 \text{ cm}^{-1}$ , respectively (Table 3). These results for the above mentioned atoms of H-Gly-Met-Gly-OH are also in accordance of experimentally determined value reported by Ivanova *et al.* (2006b). The experimentally calculated value for  $\nu(\text{C}\gamma-\text{S})$  and  $\varphi(\text{S}-\text{C}-\text{H})$  group was  $703 \text{ cm}^{-1}$  and  $1376 \text{ cm}^{-1}$ , respectively (Ivanova *et al.*, 2006a).

## CONCLUSION

The results of vibrational dynamics study concluded that the peptide, glycyl-methionyl-glycine, is an important model tripeptide to understand the mechanism of coordination of metal ions (due to their potential antitumor effect) with proteins or peptides. The vibrational dynamics of H-Gly-Met-Gly-OH can be satisfactorily interpreted from the normal modes of H-Gly-Met-Gly-OH as obtained by Wilson's GF matrix method for finite systems. The vibrational dynamics of proline-hydroxypro, pro-pro-gly and gly-pro-pro are also interpreted satisfactorily through normal modes analysis by the other researchers (Srivastava *et al.*, 2008). The spectra of those fragments can be well interpreted from normal coordinate analysis using the Urey-Bradley force field (Urey and Bradley, 1931).

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