Chapter 4

RAMAN AND IR SPECTRA OF
\( \beta \)-ALANINE AND SARCOSINE MONOPHOSPHATES
4.1 INTRODUCTION

Studies of vibrational spectra of amino acids by Raman and IR spectroscopy are useful in obtaining informations regarding the molecular conformation, dynamics of molecular motion and the nature of hydrogen bonding. IR and Raman spectra of a number of amino acids in aqueous solutions and solids have been reported [174,184-190]. Katsunosuke et al. [191] studied the Raman band intensities of some local group modes of α-glycine, L-alanine and DL-alanine crystals. Only very few studies on vibrational spectra of monophosphates of amino acids have been reported [77,80]. Structural investigations [192] of β-alanine monophosphate [BAP] and Sarcosine monophosphate [SP] suggest protonation of the amino group by a hydrogen atom of the phosphoric group and the retention of the carboxylic group in these compounds. Further, the phosphate tetrahedra are found to be considerably distorted. As these effects are expected to show up in the IR and Raman spectra, a vibrational study is performed to understand the nature of co-ordination in the orthophosphate and the carboxylic groups.

4.2 EXPERIMENTAL

The compounds are prepared by slow evaporation of an aqueous solution of β-alanine/Sarcosine and orthophosphoric acid [192] in the stoichiometric ratio at room temperature. Raman spectra [Figs.4.1 & 4.2] of the compounds at room temperature are recorded in the Stokes region of the 488.0 nm radiation from an argon ion laser using a Spex Ramalog 1403 double monochromator. The IR spectra [Figs.4.3 & 4.4] (4000-200 cm\(^{-1}\)) are obtained on Perkin-Elmer model 580 B and 983 spectrometers with the sample in KBr and in Nujol mull.

4.3 FACTOR GROUP ANALYSIS

BAP crystallises in the monoclinic system with the space group P2\(_1\)/n (C\(_{2h}\)) with four formula units in the unit cell [192]. The tetramolecular unit cell of SP is orthorhombic P2\(_1\)2\(_1\)2\(_1\)(D\(_2^4\)). All the atoms are in general sites and factor group analysis [Tables 4.1 & 4.2] predicts the distribution of the irreducible representations [25] at k=0 excluding acoustic modes as
\[ \Gamma_{\text{BAP}} = 63A_g(R)+63B_g(R)+62A_u(IR)+61B_u(IR) \]

\[ \Gamma_{\text{SP}} = 63A (R)+62B_1(R,IR)+62B_2(R,IR)+62B_3(R,IR) \]

(R-Raman active ; IR - infrared active)

The correlation diagram for the internal modes of H$_2$PO$_4$ and H$_3$PO$_4$ groups are shown in Tables 4.3-4.7.

4.4 RESULTS AND DISCUSSION

Spectra of $\beta$-alanine monophosphate

The vibrations of BAP crystal may be regarded as being composed of the following vibrations: internal vibrations of the alanine molecule and phosphate group and the external modes. The observed IR and Raman bands are tabulated in table 4.8.

Internal vibrations of $\beta$-alanine

The $\beta$-alanine molecule does not possess any symmetry and occupies a general position in the crystalline lattice. Hence all the 150 fundamental internal vibrations of the molecule are Raman and IR active. However, as the unit cell contains a large number of same type of molecular groups, the phonon energies will be closely spaced and all the predicted modes can not be observed.

In the IR spectra of BAP, the band expected around 1700 cm$^{-1}$ for an un-ionized carboxylic group is not observed. Instead, two bands have been observed at 1572 and 1603 cm$^{-1}$ which are indicative of an ionized carboxylic group. This is confirmed by the presence of $\delta$ COO' band with medium intensity at 665 cm$^{-1}$. The deprotonation of the COOH group is likely to protonate the NH$_2$ group.

In amino acids containing the NH$_3^+$ group, the stretching and bending frequencies are expected in the regions 3300-2500, 1660-1610 and 1550-1480 cm$^{-1}$ [77,177-179]. The
observation of bands at 3282, 3255 and 3045 cm$^{-1}$ in IR and at 3031 cm$^{-1}$ in Raman is indicative of the presence of NH$_3^+$ in BAP. In this compound, one band is observed in IR for each of the symmetric stretching and bending modes ($A_1$) and two bands each for the asymmetric modes ($E$). The splitting of the degenerate modes suggest that the symmetry of NH$_3^+$ is lowered from C$_{3v}$ to C$_1$ in the crystal.

The CH stretching mode of CH$_2$ group are normally found in the region 3100-2800 cm$^{-1}$ [3]. The bands observed at 3001, 2977, 2950, 2930 and 2913 cm$^{-1}$ in Raman and at 2950 and 2850 cm$^{-1}$ in IR are assigned to the stretching mode of CH$_2$. The doubling of the bending mode of CH$_2$ is probably due to the non-equivalent methylene groups. The intense band at 1020 cm$^{-1}$ in IR and 1018 cm$^{-1}$ in Raman are assigned to the symmetric stretching mode of CN. Bands due to twisting, wagging and rocking modes of CH$_2$ are also identified (Table 4.8).

**Vibrations of H$_3$PO$_4$**

The phosphate tetrahedra is distorted considerably with P-O distances 1.563, 1.498, 1.565 and 1.512 Å as the acid hydrogen atoms are bonded to the oxygen atoms of the three longest P-O bonds [192]. Hence, the vibrational assignment can be done on the basis of characteristic vibrations of H$_3$PO$_4$ group with C$_{3v}$ symmetry. A free H$_3$PO$_4$ group with C$_{3v}$ symmetry has 18 internal modes ($5A_1+3A_2+5E$). Of these, 9($3A_1+3E$) are associated with the undistorted PO$_4$ tetrahedron and the remaining 9($2A_1+A_2+3E$) with OH vibrations.

The reduction from the T$_d$ symmetry of the PO$_4^{3-}$ ion leads to a splitting of the $\nu_4(F_2)$ stretching fundamentals of PO$_4^{3-}$ to give $A$ and $E$ modes. The observation of two bands in IR [885 and 875 cm$^{-1}$] for the $A$ mode is due to correlation field effect. The splitting of the $E$ - mode into two (965 and 937 cm$^{-1}$) confirms the lowering of the symmetry of the orthophosphate group from T$_d$ to C$_1$ through C$_{3v}$ in the crystal. The splitting of the $\nu_4(F_2)$ bending mode of PO$_4^{3-}$ [Table 4.3] into three components in IR [521, 513 and 501 cm$^{-1}$] again confirms the lowering of the symmetry of the orthophosphate group. The multiplicity of bands observed for the doubly degenerate $\delta_{as}$P(OH)$_3$ mode is due to both site symmetry and correlation field effects.
Usually, P-O-H in-plane bending appears with lower intensity in IR [58,63,84]. In the present case a strong band at 1240 cm\(^{-1}\) is observed for this mode in IR. This intensity enhancement may be due to strong vibrational coupling between P-O stretching and P-O-H in-plane bending modes. The band at 816 cm\(^{-1}\) is assigned to the out-of-plane bending mode of P-O-H. The bands observed in the regions 2800-2400, 2350-1900 and 1720-1600 cm\(^{-1}\) may be assigned as trio bands which arise from the strong hydrogen bonds (O..H- O) of H\(_3\)PO\(_4\) with COO\(^-\) and NH\(_3\) with H\(_3\)PO\(_4\) (N-H...O).

**Spectra of Sarcosine Monophosphate**

The appearance of an intense band at 1700 cm\(^{-1}\) in IR for an un-ionized carboxylic group and the absence of bands corresponding to ionized carboxylic group indicate the existence of COOH group in SP.

**Vibrations of Orthophosphate ion**

In salts of aminoacids containing H\(_3\)PO\(_4\) group, the deprotonation of the H\(_3\)PO\(_4\) group is possible resulting in H\(_2\)PO\(_4^+\)[77] which may be confirmed by vibrational spectra. Table 4.5 gives the correlation of PO\(_4^4\) vibrational modes to those of H\(_3\)PO\(_4\) and H\(_2\)PO\(_4\) groups. If the group exists as H\(_2\)PO\(_4\) with C\(_{2v}\) it can be seen from the Table 4.6 that \(v_2\) (E) mode splits into two and \(v_3\) (F\(_2\)) and \(v_4\) (F\(_2\)) split into three modes each. Four bands (420,403,372 and 350cm\(^{-1}\)) have been observed in IR for the \(v_2\) (E) mode. The \(v_3\) (F\(_2\)) and \(v_4\) (F\(_2\)) modes appeared as six and four components respectively. The strong \(v_8\) PO\(_2\) (A\(_1\)) mode at 1068 cm\(^{-1}\) characteristic of H\(_2\)PO\(_4\) group with C\(_{2v}\) symmetry and intense IR band at 945 cm\(^{-1}\) corresponding to \(v_{as}\) P(OH)\(_2\) clearly indicate the possibility of existence of H\(_2\)PO\(_4^+\) ion with C\(_{2v}\) symmetry. Moreover the fact that the number of bands of the orthophosphate unit in SP is greater than that in BAP in IR also support the presence of H\(_2\)PO\(_4^+\) group in the crystal. Also, a comparison of the observed frequencies with the expected frequencies of the H\(_2\)PO\(_4^+\) for different symmetries [Table 2.2] more or less agrees with the values corresponding to C\(_{2v}\) symmetry for the H\(_2\)PO\(_4^+\) ion.

The intensity enhancement of the in-plane P-O-H bending (A\(_2\)) mode is possibly due to its strong vibrational coupling with the PO\(_2\) symmetric stretching mode. Two bands 690 cm\(^{-1}\) (strong) and 670 cm\(^{-1}\) (medium) are observed corresponding to P-O-H out-of-
plane bending probably due to vibrational coupling and correlation field effect. The observation of broad IR band around 3300 cm\(^{-1}\) in both KBr and Nujol spectra rules out the possibility of observed water in the pellet. Hence, it is assigned to the OH stretching frequency of COOH.

It is to be noted that usually deprotonation of the carboxylic group is responsible for the protonation of the amino group. Since un-ionised carboxylic group is found to exist in SP from the vibrational spectra it is evident that protonation of the amino group is at the expense of proton of the orthophosphate group. This is in agreement with the structural data [192].

4.5 CONCLUSIONS

1. The carboxylic group is deprotonated in β -alanine H\(_3\)PO\(_4\) whereas it is not in Sarcosine H\(_3\)PO\(_4\).

2. In sarcosine monophosphate the amino group is protonated at the expense of the proton from the orthophosphate group. This gives rise to the H\(_2\)PO\(_4^-\) ion.

3. The symmetry of the H\(_2\)PO\(_4\) is found to be C\(_{2v}\) in Sarcosine Monophosphate.

4. Site symmetry and correlation field effects are strong in both the compounds.
TABLE 4-1

Factor group analysis of β-alanine. H₃PO₄ (NH₂-CH₂-CH₂-COOH. H₃PO₄)

Space group P2₁/n = C₂h\(^5\); Z=Z\(^B\) =4

<table>
<thead>
<tr>
<th>Factor group species C₂h</th>
<th>NH₃ (C₁ site)</th>
<th>CH₂ (C₁ site)</th>
<th>H₃PO₄ (C₁ site)</th>
<th>Internal modes</th>
<th>External modes</th>
<th>Internal modes</th>
<th>External modes</th>
<th>O-H...O Internal modes</th>
<th>External modes</th>
<th>4C</th>
<th>8O</th>
<th>Optical modes</th>
<th>Acoustic modes</th>
<th>Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>A₉</td>
<td>6</td>
<td>3T,3R</td>
<td>6</td>
<td>6</td>
<td>6T,6R</td>
<td>9</td>
<td>9</td>
<td>3T,3R</td>
<td>3T</td>
<td>6T</td>
<td>63</td>
<td></td>
<td></td>
<td>a</td>
</tr>
<tr>
<td>B₉</td>
<td>6</td>
<td>3T,3R</td>
<td>6</td>
<td>6</td>
<td>6T,6R</td>
<td>9</td>
<td>9</td>
<td>3T,3R</td>
<td>3T</td>
<td>6T</td>
<td>63</td>
<td></td>
<td></td>
<td>a</td>
</tr>
<tr>
<td>A₁ₙ</td>
<td>6</td>
<td>3T,3R</td>
<td>6</td>
<td>6</td>
<td>6T,6R</td>
<td>9</td>
<td>9</td>
<td>3T,3R</td>
<td>3T</td>
<td>6T</td>
<td>63</td>
<td></td>
<td>-1</td>
<td>f</td>
</tr>
<tr>
<td>B₁ₙ</td>
<td>6</td>
<td>3T,3R</td>
<td>6</td>
<td>6</td>
<td>6T,6R</td>
<td>9</td>
<td>9</td>
<td>3T,3R</td>
<td>3T</td>
<td>6T</td>
<td>63</td>
<td></td>
<td>-2</td>
<td>f</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>12T,12R</td>
<td>24</td>
<td>24</td>
<td>24T,24R</td>
<td>36</td>
<td>36</td>
<td>12T,12R</td>
<td>12T</td>
<td>24T</td>
<td>252</td>
<td></td>
<td>-3</td>
<td></td>
</tr>
</tbody>
</table>
TABLE 4.2
Factors group analysis of Sarcosine H₃PO₄ [CH₃CH₂ NHCOOH. H₃PO₄]
Space group p2₁2₁2₁ = D₂⁴ ; Z = Z'B = 4

<table>
<thead>
<tr>
<th>Factor group species D₂</th>
<th>C₁⁺(C₁ Site)</th>
<th>CH₂ (C₁ Site)</th>
<th>NH₂ (C₁ Site)</th>
<th>H₂PO₄ (C₁ site)</th>
<th>Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Internal modes</td>
<td>External modes</td>
<td>Internal modes</td>
<td>External modes</td>
<td>PO₄ Internal vibrations</td>
</tr>
<tr>
<td>A</td>
<td>6 3T, 3R</td>
<td>3 3T, 3R</td>
<td>9 6 3T, 3R</td>
<td>3T 6T 3T 63</td>
<td>a</td>
</tr>
<tr>
<td>B₁</td>
<td>6 3T, 3R</td>
<td>3 3T, 3R</td>
<td>9 6 3T, 3R</td>
<td>3T 6T 3T 63</td>
<td>-1</td>
</tr>
<tr>
<td>B₂</td>
<td>6 3T, 3R</td>
<td>3 3T, 3R</td>
<td>9 6 3T, 3R</td>
<td>3T 6T 3T 63</td>
<td>-1</td>
</tr>
<tr>
<td>B₃</td>
<td>6 3T, 3R</td>
<td>3 3T, 3R</td>
<td>9 6 3T, 3R</td>
<td>3T 6T 3T 63</td>
<td>-1</td>
</tr>
<tr>
<td></td>
<td>24 12T, 12R</td>
<td>12 12T, 12R</td>
<td>36 24 12T, 12R</td>
<td>12T 24T 12T 252</td>
<td>3</td>
</tr>
</tbody>
</table>
TABLE 4.3

Correlation scheme for the internal vibrations of PO$_4$ in β-alanine monophosphate

<table>
<thead>
<tr>
<th>PO$_4$ ion Symmetry</th>
<th>H$_3$PO$_4$ ion symmetry</th>
<th>Site symmetry</th>
<th>Factor group symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Td</td>
<td>C$_3v$</td>
<td>C$_1$</td>
<td>C$2h$</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\nu(P-O) & \quad A_1 \quad \text{E} \\
\delta_{as} \ P(OH) & \quad A_1 \quad \text{E} \\
\nu_s \ P(OH) & \quad A_1 \quad \text{E} \\
\end{align*}
\]
TABLE 4.4
Correlation scheme for the internal vibrations of $\text{H}_3\text{PO}_4$
group in $\beta$ - alanine monophosphate

<table>
<thead>
<tr>
<th>H$_3$PO$<em>4$ symmetry C$</em>{3v}$</th>
<th>Site symmetry C$_1$</th>
<th>Factor group symmetry C$_{2h}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$PO_4$ Vibrations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12  $A_1$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24  $E$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$OH$ Vibrations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8   $2A_1$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4   $A_2$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24  $3E$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
TABLE 4.5

Correlation scheme for the PO₄ vibrations to the internal modes of H₂PO₄ and H₂PO₄ groups

<table>
<thead>
<tr>
<th>PO₄ ion symmetry</th>
<th>H₃PO₄ ion symmetry</th>
<th>H₂PO₄ ion symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Td</td>
<td>C₃v</td>
<td>C₂v</td>
</tr>
</tbody>
</table>

- (v₁) A₁ → A₁
- (v₂) E → E → A₁, A₂
- (v₃) F₂ → A₁, E → B₁, B₂
- (v₄) F₂ → A₁, E → B₁, B₂
TABLE 4.6

Correlation scheme for the internal vibrations of PO₄ ion in
Sarcosine monophosphate

<table>
<thead>
<tr>
<th>PO₄ ion symmetry</th>
<th>H₂PO₄ ion symmetry</th>
<th>Site symmetry</th>
<th>Factor group symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tₐ</td>
<td>Cᵥ</td>
<td>C₁</td>
<td>D₂</td>
</tr>
</tbody>
</table>

$$
\begin{align*}
A₁ & \rightarrow A₁ & A & \rightarrow A (R) & B₁ + B₂ + B₃ (R, IR) \\
E & \rightarrow A₁ & A & \rightarrow A (R) & B₁ + B₂ + B₃ (R, IR) \\
F₂ & \rightarrow A₁ & A & \rightarrow A (R) & B₁ + B₂ + B₃ (R, IR) \\
F₂ & \rightarrow B₁ & A & \rightarrow A (R) & B₁ + B₂ + B₃ (R, IR) \\
F₂ & \rightarrow B₂ & A & \rightarrow A (R) & B₁ + B₂ + B₃ (R, IR)
\end{align*}
$$
TABLE 4.7
Correlation scheme for the internal vibrations of H$_2$PO$_4$ ion in Sarcosine monophosphate

<table>
<thead>
<tr>
<th>$f^2$</th>
<th>H$_2$PO$<em>4$ ion symmetry $C</em>{2v}$</th>
<th>Site symmetry $C_1$</th>
<th>Factor group symmetry $D_2$</th>
</tr>
</thead>
</table>

**PO$_4$ Vibrations**

| 16   | 4A$_1$                           | A 9                 |
| 4    | A$_2$                            | B$_1$ 9             |
| 8    | 2B$_1$                           | B$_2$ 9             |
| 8    | 2B$_2$                           | B$_3$ 9             |

**OH Vibrations**

<p>| 8    | 2A$_1$                           | A 6                 |
| 4    | A$_2$                            | B$_1$ 6             |
| 8    | 2B$_1$                           | B$_2$ 6             |
| 4    | B$_2$                            | B$_3$ 6             |</p>
<table>
<thead>
<tr>
<th></th>
<th>( \beta ) - Alanine Phosphate</th>
<th>Sarcosine Monophosphate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Raman</strong></td>
<td><strong>IR</strong></td>
</tr>
<tr>
<td>3031 m</td>
<td>3282 s</td>
<td>( \nu_{\text{as}} \text{NH}_3^+ )</td>
</tr>
<tr>
<td></td>
<td>3255 s</td>
<td>( \nu_{\text{s}} \text{NH}_3^+ )</td>
</tr>
<tr>
<td>3001 s</td>
<td>3047 m</td>
<td></td>
</tr>
<tr>
<td>2977 vs</td>
<td>3037 m</td>
<td></td>
</tr>
<tr>
<td>2950 vvs</td>
<td>3017 s</td>
<td>( \nu_{\text{as}} \text{CH}_2 )</td>
</tr>
<tr>
<td>2930 w</td>
<td>2975 v s</td>
<td>( \nu_{\text{as}} \text{CH}_2 )</td>
</tr>
<tr>
<td>2813 m</td>
<td>2950 ?</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2850 w</td>
<td></td>
</tr>
<tr>
<td>2612 w</td>
<td></td>
<td>Trio bands</td>
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<tr>
<td>2562 w</td>
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<td>overtones</td>
</tr>
<tr>
<td>2478 m</td>
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<td>combinations</td>
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<tr>
<td>1904 w</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1808 w</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1707 v, b</td>
</tr>
<tr>
<td>1658 w</td>
<td>1675 s</td>
<td>( \delta_{\text{as}} \text{NH}_3^+ )</td>
</tr>
<tr>
<td></td>
<td>1642 m</td>
<td></td>
</tr>
<tr>
<td>1603 w</td>
<td>1572 w</td>
<td>( \nu_{\text{as}} \text{COO}^- )</td>
</tr>
<tr>
<td>1510 s</td>
<td></td>
<td>( \delta_{\text{s}} \text{NH}_3^+ )</td>
</tr>
<tr>
<td>1469 w</td>
<td>1472 m</td>
<td>( \delta_{\text{s}} \text{CH}_2 )</td>
</tr>
<tr>
<td></td>
<td>1462 sh</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1405 m</td>
<td>1408 s</td>
<td>( \nu_{\text{s}} \text{COO}^- )</td>
</tr>
<tr>
<td></td>
<td>1380 m</td>
<td>( \delta \text{C-C-H} )</td>
</tr>
<tr>
<td>1336</td>
<td>1284 m</td>
<td>( \omega \text{CH}_2 ), ( \iota \text{CH}_2 )</td>
</tr>
<tr>
<td>1263 s</td>
<td>1240 s</td>
<td>( \delta \text{P-O-H in } \text{-plane} )</td>
</tr>
<tr>
<td>1234 w</td>
<td>1155 m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1140 vs</td>
<td></td>
</tr>
<tr>
<td>1120 vs</td>
<td>1220 vs</td>
<td>v PO (A(_1))</td>
</tr>
<tr>
<td>1063 w</td>
<td>1065 w</td>
<td></td>
</tr>
<tr>
<td>1018 w</td>
<td>1020 vs</td>
<td>( \nu_{\text{C}} \text{CN} )</td>
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<td></td>
<td>995 sh</td>
<td>( \nu \text{CH}_2 )</td>
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<tr>
<td></td>
<td>982 w</td>
<td>( \nu \text{CH}_2 )</td>
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### TABLE 4.8
Vibrational spectral data (in cm⁻¹) and band assignments* of BAP and SP

<table>
<thead>
<tr>
<th>Raman</th>
<th>IR</th>
<th>Assignment</th>
<th>Raman</th>
<th>IR</th>
<th>Assignment</th>
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<tbody>
<tr>
<td>943 w</td>
<td>965 vvs</td>
<td>$\nu_{as} P(OH)_3$ (E)</td>
<td>945 vvs</td>
<td>$\nu_{as} P(OH)_2$ (B₁)</td>
<td></td>
</tr>
<tr>
<td>884 vs</td>
<td>885 sh</td>
<td>$\nu_{s} P(OH)_3$ (A₁)</td>
<td>921 s</td>
<td>920 m</td>
<td>r CH₃, rCH₂</td>
</tr>
<tr>
<td>830 vw</td>
<td>830 m</td>
<td>$\nu_{s} C-C$</td>
<td>884 m</td>
<td>885 s</td>
<td>vs P(OH)_2 (A₁)</td>
</tr>
<tr>
<td>816 m</td>
<td>$\gamma P-OH$ out of plane</td>
<td>828 m</td>
<td>r CH₃</td>
<td></td>
<td></td>
</tr>
<tr>
<td>721 m</td>
<td>$\delta COO^-$</td>
<td>690 s</td>
<td>$\gamma POH$ out of plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>665 m</td>
<td>$\omega COO^-$</td>
<td>564 s</td>
<td>541 s</td>
<td>$\delta sPO_2$</td>
<td></td>
</tr>
<tr>
<td>587 vw</td>
<td>543 s</td>
<td>rCOO⁻</td>
<td>485 m</td>
<td>475 w</td>
<td>$\delta CNC$</td>
</tr>
<tr>
<td>540 w</td>
<td>521 m</td>
<td>$\delta_{s} P (OH)_3$ (A₁)</td>
<td>420 vw</td>
<td>$\delta s P(OH)_2$</td>
<td></td>
</tr>
<tr>
<td>513 m</td>
<td>$\gamma P(OH)_3$ (E)</td>
<td>403 w</td>
<td>372 m</td>
<td>t PO₂</td>
<td></td>
</tr>
<tr>
<td>501 vs</td>
<td>390 w</td>
<td>300 w</td>
<td>350 w</td>
<td></td>
<td></td>
</tr>
<tr>
<td>420 vw</td>
<td>400 s</td>
<td>387 vw</td>
<td>366 vw</td>
<td></td>
<td></td>
</tr>
<tr>
<td>386 sh</td>
<td>$\delta_{as} P(OH)_3$ (E)</td>
<td>288 m</td>
<td>t CH₂</td>
<td>282 sh</td>
<td>t CH₃, t CH₂</td>
</tr>
<tr>
<td>366 w</td>
<td>288 m</td>
<td>t CH₂</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Relative intensities: v= very; s= strong; m= medium; w= weak; sh= shoulder; br=broad; ν = stretching; δ=bending; as=antisymmetric; s=symmetric; ω= wagging; t= twisting; r= rocking
Fig. 4.1 RAMAN SPECTRUM OF $\beta$ ALANINE $\text{H}_3\text{PO}_4$ IN THE 50 - 3500 $\text{cm}^{-1}$ REGION
Fig. 4.3 IR SPECTRUM OF $\beta$-ALANINE $\text{H}_3\text{PO}_4$ IN THE 200-4000 cm$^{-1}$ REGION
Fig. 4.4 IR SPECTRUM OF SARCOSINE $\text{H}_3\text{PO}_4$ IN THE 200 - 4000 $\text{cm}^{-1}$ REGION