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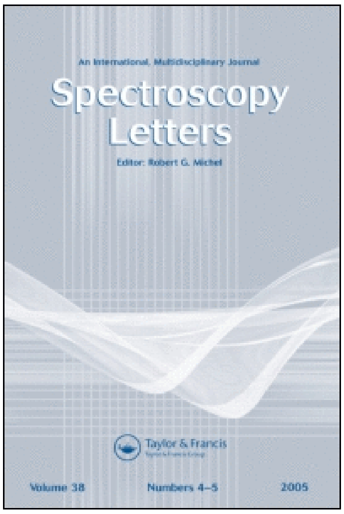

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# The Vibrational Spectra of Crystalline Sodium Pyruvate

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# THE VIBRATIONAL SPECTRA OF CRYSTALLINE SODIUM PYRUVATE*

Keywords: Sodium Pyruvate, Infrared Spectra, Raman Spectra

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The pyruvate ion is a biochemically important molecule, but its vibrational spectra appear not to have been studied previously in any detail. In view of this, and our interest in the vibrational spectra of simple organic acids and their derivatives, it seemed desirable to carry out a detailed analysis of the vibrational spectra of this ion. Sodium pyruvate is only sparingly soluble in water at ambient temperatures and is insoluble in common organic solvents. The spectra were therefore recorded on crystals which were purchased from Aldrich Chemical Company, recrystallized from distilled water and washed with $CCl_4$. The crystal structure of sodium pyruvate has been determined previously by x-ray diffraction[1]. The molecule crystallizes in the $P2_1/a$ space group with four molecules per unit cell. The $CO_2^-$ group is rotated 18° from the plane containing the other heavy atoms.

Infrared spectra were recorded as Nujol and hexachlorobutadiene mulls on a Perkin-Elmer Model 180 infrared spectrophotometer. Raman spectra of the crystals were recorded directly on a Cary Model 81 Raman spectrometer equipped with a Coherent Radiation Model CR-3 argon laser using the 488 nm line. A typical mixed mull infrared spectrum is reproduced in Figure 1 and a typical Raman spectrum is reproduced in Figure 2. The observed data, along with their proposed assignments, are given in Table 1.

Observation of the spectra immediately reveals that many of the infrared bands do not agree with the Raman bands within experimental error, even though the molecule does not contain a center of symmetry. Such behavior has been previously noted in the spectra of salts and discussed in some detail[2]. It is apparently due to crystallization in centrosymmetric space groups (such as $P2_1/a$) and the strong intermolecular interactions of the ions. This leads to exceptionally large crystal splittings in these compounds.

The detailed assignment has been carried out using the standard group frequencies available[3,4] and by comparison with the vibrational assignment of methyl pyruvate previously published[5] and those for a number of salts of simple carboxylic acids[2].

Table 1 lists the assignments of methyl pyruvate[5] for the $CH_3CO$-portion of the molecule for comparison with those proposed for the salt. It is seen that frequencies are in close agreement except for one $CH_3$ antisymmetric bending frequency (1419 vs 1381 $cm^{-1}$) and some of the skeletal bending vibrations, which are known to be highly characteristic vibrations of the entire molecule. It is probable that the 1419 $cm^{-1}$ bending mode has been shifted to lower frequency in the salt because of Fermi Resonance with the strong $CO_2$ symmetric stretching frequency at 1409 $cm^{-1}$. This mode does not occur in methyl pyruvate.

The remainder of the fundamental modes are due to the $CO_2^-$ portion of the molecule and compare well with similar modes in other salts except for the low frequency modes. This is again presumably due to the highly

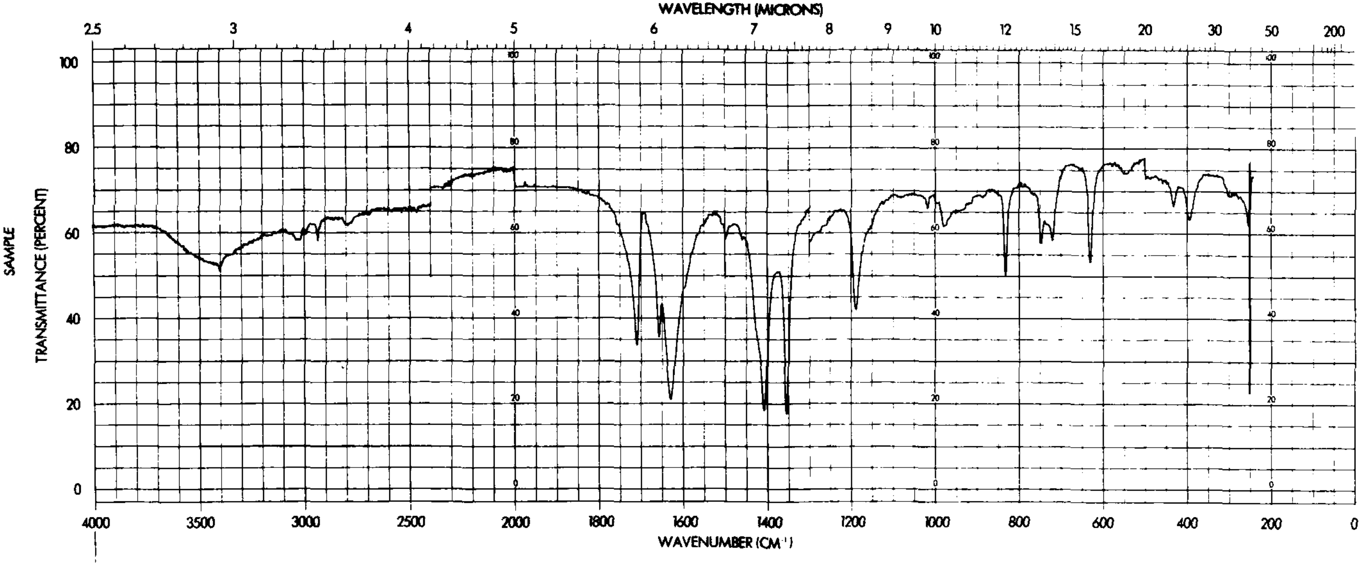

Figure 1. Typical Mixed Mull Infrared Spectrum of Sodium Pyruvate (a small amount of water is retained by the salt as evidenced by the weak broad band near 3400 $cm^{-1}$).

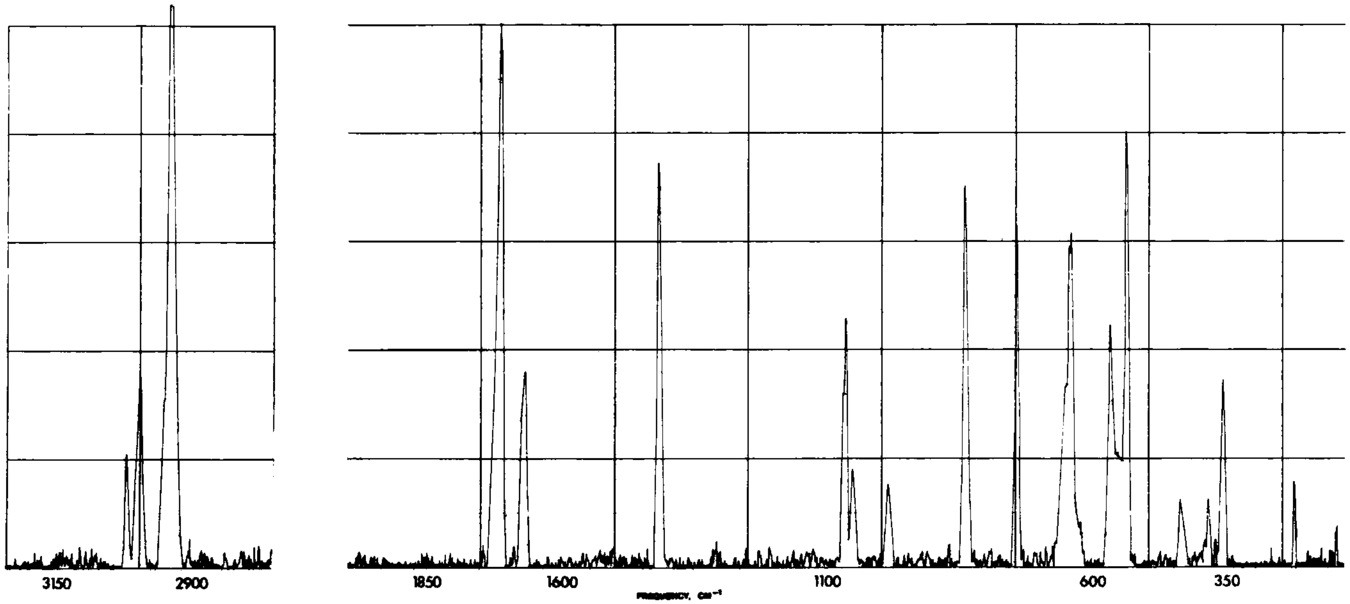

Figure 2. Typical Raman Spectrum of Crystalline Sodium Pyruvate. (The spectrum has been redrawn to give a zero baseline).

## TABLE 1

### The Observed Vibrational Spectra of Sodium Pyruvate (in $cm^{-1}$) and Their Tentative Assignment

| Infrared | Raman | Assignment | Corresponding Assignment of Methyl Pyruvate[5] |
|---|---|---|---|
| 3026 w | 3015 w | $\nu CH_3$ asym | 3008 |
| 2991 w | 2989 wm | $\nu CH_3$ asym | 2981 |
| 2922 w | 2932 s | $\nu CH_3$ sym | 2929 |
| 2340 w | | 1709+629 | |
| 1928 vw | | 1709+219 | |
| 1709 s | 1703 s | $\nu C=O$ | 1739 |
| 1657 m-s | 1659 m | $\nu CO_2$ asym | |
| 1628 m | | 1407 219 | |
| 1597 w | | 1381+219 | |
| 1505 w | | 1381+120 | |
| 1467 w | | 832+629 | |
| 1430 w | | $\delta CH_3$ sym | 1425 |
| 1407 m | 1409 m-s | $\nu CO_2$ sym | |
| 1381 w | | $\delta CH_3$ asym | 1419 |
| 1354 s | 1369 m | $\delta CH_3$ sym | 1356 |
| 1190 m | | 832+354 | |
| | 1058 m | $\delta CH_3$ rock | 1056 |
| 1016 w | | $\delta CH_3$ rock | 1017 |
| | 1044 w-m | $\nu C-C$ | 1000 |
| 979 w | | 629+354 | |
| | 978 w | 636+354 | |
| 882 w | | | |
| 832 m | 837 s | $\nu CH_3-C$ | 827 |
| 749 w-m | 738 m-s | $\delta CO_2$, scissors | |
| 629 w-m | 636 m-s | $\delta CO_2$, wag | |
| | 563 m | $\gamma$ skeleton | 546 |
| 545 w | 532 s | $\delta$ skeleton | 403 |
| | 438 w | 2x221 | |
| 432 w | | 2x219 | |
| 395 m | 384 w | $\delta$ skeleton | 340 |
| 354 w | 354 w | $\gamma CO_2$, rock | |
| 219 w | 221 w | $CO_2$ torsion ? | |
| 120 w | | $CH_3$ torsion? | |

s = strong, v = very, m = medium, w = weak, $\nu$ = stretch, $\delta$ - in-plane bend, $\gamma$ = out-of-plane bend, sym = symmetric, asym = antisymmetric characteristic nature of low frequency skeletal modes. The two lowest frequency modes (219 and 120 $cm^{-1}$) are tentatively assigned as torsional modes but may be due to lattice vibrations.

## ACKNOWLEDGMENT

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