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# INFRARED SPECTRUM OF ACETONITRILE-$^{15}$N

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## ABSTRACT

Acetonitrile-$^{15}$N has been synthesized from ammonium chloride with a 99.4% $^{15}$N isotopic content. The IR spectrum of the liquid has been recorded in the range 10,000 —20 cm$^{-1}$ and some new assignments have been proposed particularly in the range 10,000 —4,000 cm$^{-1}$. The spectrum of the gas has been recorded in the range 4,000—200 cm$^{-1}$ and $\nu_5$ and $\nu_7$ have been analyzed as well as the $\nu_6$, $\nu_7 + \nu_8$ Fermi resonant band system. Molecular parameters suitable for force constant refinements have been calculated.

## INTRODUCTION

Prior to this work some work has been carried out on the vibrational and rotation—vibration spectrum of acetonitrile ($CH_3CN$) and its isomers $CD_3CN$, $^{13}CH_3CN$ and $CH_3{}^{13}CN$ [1—18]. Molecular structure has been established by microwave absorption spectroscopy of $CH_3CN$ and its partially deuterated derivatives [19—20], IR spectroscopy [21] and electron diffraction [22—23]. Likewise, the pure rotation spectra of $CH_3C^{14}N$ and $CH_3C^{15}N$ have been investigated in the vibrational ground level and in some excited levels [24—27] In this work we have investigated the IR spectrum of $CH_3C^{15}N$ as a pure liquid and in the gas phase. We have proposed some new assignments in the spectrum of the liquid especially in the range 10,000—4,000 cm$^{-1}$ where only overtone and combination bands appear. In the spectrum of the gas the $\nu_5$ and $\nu_7$ perpendicular bands have been resolved and band centres as well as Coriolis $\zeta$-constants have been calculated. On the other hand, we have analysed the Fermi resonance between $\nu_6$ and $\nu_7 + \nu_8$ according to the method described by Duncan et al. [15], obtaining unperturbed band centres and $\zeta$-constants as well as the parameter $k_{678}$ which accounts for the interaction.

## EXPERIMENTAL

Acetonitrile-$^{15}$N has been synthesized using a sample of ammonium chloride with a 99.4% $^{15}$N isotopic content as a source of this isotope. As an

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intermediate we synthesized acetamide according to the method described in ref. 28 and thereafter acetonitrile was obtained by distillation of the amide with $P_2O_5$ and purified by redistillation with $K_2CO_3$ and $Na_2SO_4$. The purity of the sample was checked by inspection of its IR spectrum and by comparison with that of a sample of acetonitrile Carlo Erba RS reagent for spectrophotometry. Infrared spectra of the liquid were recorded on a PE-125 spectrophotometer in the range 10,000—400 $cm^{-1}$ and on a Beckman FS720 Fourier spectrophotometer in the range 400—20 $cm^{-1}$. The records from liquid samples were obtained with 0.1 and 1.0 mm pathlength cells in the range 10,000—4,000 $cm^{-1}$, 0.025 mm in the range 4,000—400 $cm^{-1}$ and 1.0 mm in the range 400—20 $cm^{-1}$. Spectra of gas samples were recorded on a PE225 spectrophotometer in the range 4,000—200 $cm^{-1}$ using a continuous flow chart recorder. Standard 12 cm pathlength gas cells were used with variable vapor pressure up to saturation depending on the intensities of the bands. Standard gases were used for calibration according to ref. 29, several measurements were made on each record and mean values were obtained for the wavenumbers of the recorded peaks.

## RESULTS

Table 1 summarizes our experimental results concerning the wavenumbers of IR absorption bands of liquid acetonitrile and the isotopic shifts due to $^{15}N$. It also shows Raman shifts and depolarization ratios according to refs. 13 and 8 respectively. Table 2 summarizes the wavenumbers of the bands recorded in the range 10,000—4,000 $cm^{-1}$ as well as their isotopic shifts. Experimental data for acetonitrile in the gas phase are shown in Table 3. Wavenumbers for $\nu_1$, $2\nu_6$, $2\nu_3$, $\nu_3 + \nu_6$, $\nu_2$, $\nu_4$ and $2\nu_8$ were measured directly as the respective $Q$ branch maxima of parallel bands. Wavenumbers of $\nu_3$ fundamentals were estimated from perturbations observed in the structure of $\nu_6$ fundamentals. The isotopic shift for $\nu_8$ was calculated from that of $2\nu_8$ by assuming $\Delta\nu_8 = 1/2\Delta 2\nu_8$, provided that $\nu_8$ has not been resolved. Concerning perpendicular bands, $\nu_6$ and $\nu_7 + \nu_8$ were obtained from the analysis of the Fermi resonance that they undergo and $\nu_5$, $\nu_7$ were determined by rotational analysis of $Q$ branch maxima in terms of the usual quadratic expression in $K$. The accuracy of wavenumbers when sharp $Q$ branch maxima were measured is ±0.1 $cm^{-1}$ or better.

## DISCUSSION

*Spectrum of liquid acetonitrile-$^{15}N$.* The assignments we have proposed agree with almost all those of previous workers but some doubts concerning the assignment of $\nu_6$ have been elucidated, the true nature of $\nu_4$ has been experimentally checked and several combination and overtone bands have been assigned for the first time. Concerning the vibration $\nu_4$ the important isotopic shift it undergoes towards lower frequencies has to be stressed. It is evident that this vibration involves the three axial atoms CCN simultaneously as predicted by ref. 12. The observed isotopic shift of $\nu_4$ proves that we have to

TABLE 1

Summary of vibrational frequencies, $^{15}$N isotopic shifts and assignments for acetonitrile in the liquid state ($\nu$ and $\Delta\nu$ in cm$^{-1}$)

| Raman data | | Infrared data | | | Assignments |
|---|---|---|---|---|---|
| $\Delta\nu^{a}$ | $\rho_n^{b}$ | $\nu^{0}$ | $I$ | $\nu^{i} - \nu^{0}$ | |
| 380 | 0.86 | 379 | s | −2(calc.) | $\nu_8$; $\beta(CCN)E$ |
| 674 | 0.46 | — | — | — | — |
| 754 | 0.51 | 752 | s | −4 | $2\nu_8$; $A_1 + E$ |
| 920 | 0.17 | 918 | s | −8 | $\nu_4$; $\nu(CC)A_1$ |
| 1044 | — | 1040 | s | 0 | $\nu_7$; $r(CH_3)E$ |
| 1378 | 0.52 | 1378 | vs | −2 | $\nu_3$; $\delta_s(CH_3)A_1$ |
| 1414 | — | 1420 | m | −4 | $\nu_7 + \nu_8$; $A_1 + E^{c}$ |
| 1449 | 0.85 | 1444 | sb | 0 | $\nu_6$; $\delta_{as}(CH_3)E$ |
| 1558 | — | — | — | — | — |
| — | — | 1828 | w | −18 | $2\nu_4$; $A_1$ |
| — | — | 2070 | w | 0 | $2\nu_7$; $A_1 + E$ |
| 2197 | — | 2200 | w | −22 | $2\nu_4 + \nu_8$; $E$ |
| 2248 | 0.20 | 2256 | vs | −31 | $\nu_2$; $\nu(CN)A_1$ |
| 2289 | 0.26 | 2290 | s | −10 | $\nu_3 + \nu_4$; $A_1$ |
| — | — | 2410 | m | 0 | $\nu_3 + \nu_7$; $E$ |
| 2460 | — | 2480 | w | 0 | $\nu_6 + \nu_7$; $A_1 + E^{c}$ |
| — | — | 2630 | m | −35 | $\nu_2 + \nu_8$; $E$ |
| 2644 | — | — | — | — | — |
| 2736 | — | — | — | — | — |
| 2841 | — | — | — | — | — |
| 2887 | p | — | — | — | — |
| 2942 | 0.09 | 2945 | s | 0 | $\nu_1$; $\nu_s(CH_3)A_1$ |
| 2999 | 0.86 | 3000 | s | 0 | $\nu_5$; $\nu_{as}(CH_3)E$ |
| — | — | 3165 | s | −35 | $\nu_2 + \nu_4$; $A_1$ |
| — | — | 3200 | w | −20 | $2\nu_4 + \nu_3$; $A_1$ |
| — | — | 3970 | w | 0 | $\nu_1 + \nu_7$; $E$ |

[a]See ref. 11. [b]See ref. 7. [c]See the text, $A_2$ is omitted.

consider two coupled vibrations, $\nu_2$ in which $\nu$(CN) takes part predominantly and $\nu_4$ in which $\nu$(CC) does. With respect to $\nu_6$ we believe that it must be assigned to the strong band recorded at 1444 cm$^{-1}$ in the spectrum of the liquid instead of that at 1420 cm$^{-1}$ to which it was assigned in ref. 14, because the first of these bands does not shift at all towards lower frequencies as is to be expected for a $\delta_{as}(CH_3)$ vibration. The second of the mentioned bands exhibits a non-zero isotopic shift and therefore its assignment is more in accordance with the combination $\nu_7 + \nu_8$ proposed in ref. 13. On the other hand, the symmetry of the level $\nu_7 + \nu_8$ must be $A_1 + A_2 + E$ but the allowed transitions both in the Raman and IR spectra are those from the ground state to those of symmetry $A_1$ and $E$, therefore, it is not relevant to include $A_2$ in the assignment. The same happens for the combination $\nu_6 + \nu_7$, the assignment of which is confirmed by its zero isotopic shift. The behaviour of the other bands included in Table 1 confirms the assignments proposed by

TABLE 2

Combination and overtone bands in the IR spectrum of acetonitrile in the liquid state. Range 10,000—4,000 cm$^{-1}$

| $\nu^0$ | $I$ | $\nu^i - \nu^0$ | Assignments | $\nu^0$ | $I$ | $\nu^i - \nu^0$ | Assignments |
|---|---|---|---|---|---|---|---|
| 4026 | s | 0 | $\nu_5 + \nu_7; A_1 + E^{a}$ | 5667 | vw | — | — |
| 4319 | m | —2 | $\nu_1 + \nu_3; A_1$ | 5701 | vw | — | — |
| 4365 | vs | —2 | $\nu_3 + \nu_5; E$ | 5827 | s | 0 | $2\nu_1; A_1$ |
| 4392 | m | 0 | $\nu_1 + \nu_6; E$ | 5950 | s | 0 | $2\nu_5; A_1 + E$ |
| 4437 | vs | 0 | $\nu_5 + \nu_6; A_1 + E^{a}$ | 5980 | sh | — | — |
| 4689 | vvw | — | — | 6266 | vw | — | — |
| 4774 | vw | — | — | 6845 | wb | — | $2\nu_1 + \nu_7; E$ or |
| 4938 | vvw | — | — | | | | $2\nu_5 + \nu_4; A_1 + E$ |
| 4992 | m | 0 | $2\nu_7 + \nu_1; A_1 + E$ | 7194 | w | — | $2\nu_1 + \nu_3; A_1$ |
| 5058 | w | 0 | $2\nu_7 + \nu_5; A_1 + 2E^{a}$ | 7284 | w | — | $2\nu_5 + \nu_3; A_1 + E$ |
| 5194 | m | —30 | $\nu_1 + \nu_2; A_1$ | 7369 | vvw | — | — |
| 5248 | m | —30 | $\nu_2 + \nu_5; E$ | 7410 | vvw | — | — |
| 5378 | vw | — | — | 8517 | w | — | $2\nu_1 + 2\nu_3; A_1$ |
| — | — | — | — | 8592 | w | — | $2\nu_3 + 2\nu_5; A_1 + E$ |

[a] $A_2$ is omitted.

TABLE 3

Summary of frequencies, $^{15}$N isotopic shifts and assignments for acetonitrile in the gas phase. ($\nu_0$ refers to $CH_3CN$)

| $\nu_0$ | $\Delta\nu$ | Assignment | $\nu_0$ | $\Delta\nu$ | Assignment |
|---|---|---|---|---|---|
| 3009.16 | 0 | $\nu_5; \nu_{as}(CH_3)E$ | 1448.03 | 0.18 | $\nu_6; \delta_{as}(CH_3)E$ |
| 2953.92 | 0.16 | $\nu_1; \nu_s(CH_3)A_1$ | 1410.2 | 1.4 | $\nu_7 + \nu_8; A_1 + E^{b}$ |
| 2868.62 | 0.13 | $2\nu_6; A_1 + E$ | 1390.0 | 0 | $\nu_3; \delta_s(CH_3)A_1$ |
| 2757.09 | [a] | $2\nu_3; A_1$ | 1040.79 | 0.11 | $\nu_7; r(CH_3)E$ |
| 2305.42 | 12.88 | $\nu_3 + \nu_4; A_1$ | 919.92 | 8.71 | $\nu_4; \nu(CC)A_1$ |
| 2266.45 | 26.15 | $\nu_2; \nu(CN)A_1$ | 716.77 | 5.22 | $2\nu_8; A_1 + E$ |
| | | | 364.71 | 2.61 | $\nu_8; \delta(CCN)E$ |

[a] Not observed for $CH_3C^{15}N$. [b] $A_2$ is omitted.

previous authors. In addition $2\nu_4$, $2\nu_7$, $2\nu_4 + \nu_3$ and $\nu_1 + \nu_7$ have been assigned. Finally, we propose assignments for the bands recorded in the range 10,000—4,000 cm$^{-1}$ which are summarized in Table 2.

*Spectrum of acetonitrile-$^{15}$N in the gas phase.* The analysis of $\nu_5$ and $\nu_7$ has been carried out according to the usual quadratic expression in $K$. Experimental data have been adjusted to fit $\nu_0^{sub} = a + 2bM + cM^2$ by a least squares method. For $\nu_5$ the calculated parameters are as follows

$$a = \nu_5^0 + A_5(1 - 2\zeta_5^z) - B_5 = 3013.38 \text{ cm}^{-1}$$
$$b = A_5(1 - \zeta_5^z) - B_5 = 4.6067 \text{ cm}^{-1}$$
$$c = (A_5 - A_0) - (B_5 - B_0) = -0.0338 \text{ cm}^{-1}$$

Assuming $A_0 = 5.280$ cm$^{-1}$ [19] and $B_0 = B_5 = 0.2992$ cm$^{-1}$ [26], we obtained $A_5 = 5.2462$ cm$^{-1}$, $\zeta_5^z = 0.065 \pm 0.02$ and $\nu_5^0 = 3009.11 \pm 0.05$ cm$^{-1}$. On the other hand, we found the following parameters for $\nu_7$; $a = 1042.12$ cm$^{-1}$, $b = 2.7824$ cm$^{-1}$ and $c = 0.0318$ cm$^{-1}$, which by using the same values for $A_0$ and $B_0 = B_7$ yield, $A_7 = 5.3118$ cm$^{-1}$, $\zeta_7^z = 0.420 \pm 0.01$ and $\nu_7^0 = 1040.68$ cm$^{-1}$.

The analysis of the $\nu_6$, $\nu_7 + \nu_8$ Fermi resonance band system has been carried out according to ref. 15. Wavenumbers for $Q$ branches were measured in terms of the $Q$ branch maxima for symmetrical branches but in terms of the leading edge for those $Q$ branches more or less strongly degrading because of the Coriolis interaction with the parallel fundamental $\nu_3$. The change in the sense of the degradation enabled us to assign the weak $Q$ branch of $\nu_3$ at 1390 cm$^{-1}$. Observed and calculated wavenumbers for $Q$ branch maxima are collected in Table 4. The Fermi resonance parameter $k_{678}$ has been obtained graphically from the minimum of a plot of $\nu_K^+ - \nu_k^-$ vs. $K$, and accepted to be $30.82 \pm 0.3$ cm$^{-1}$. The following expressions were evaluated as described in ref. 15

TABLE 4

Observed and calculated $Q$ branch wavenumbers for the $\nu_6$, $\nu_7 + \nu_8$ resonating diad of acetonitrile-$^{15}$N

| | $\nu^+$ | | | $\nu^-$ | | |
|---|---|---|---|---|---|---|
| | Obs. | Calc. | Δ | Obs. | Calc. | Δ |
| $^{R}Q_{12}$ | — | | | 1604.15 | 1604.59 | —0.44 |
| $^{R}Q_{11}$ | — | | | 1592.06 | 1592.19 | —0.13 |
| $^{R}Q_{10}$ | — | | | 1579.77 | 1579.65 | +0.12 |
| $^{R}Q_{9}$ | — | | | 1567.26 | 1566.95 | +0.31 |
| $^{R}Q_{8}$ | — | | | 1554.17 | 1554.03 | +0.14 |
| $^{R}Q_{7}$ | 1598.53 | 1598.65 | —0.12 | 1541.21 | 1540.85 | +0.37 |
| $^{R}Q_{6}$ | 1575.86 | 1575.99 | —0.13 | 1527.49 | 1527.27 | +0.22 |
| $^{R}Q_{5}$ | 1554.17 | 1553.82 | +0.35 | 1513.31 | 1513.10 | +0.21 |
| $^{R}Q_{4}$ | 1532.08 | 1532.49 | —0.41 | 1497.86 | 1497.97 | —0.11 |
| $^{R}Q_{3}$ | 1512.37 | 1512.54 | —0.17 | 1481.13 | 1481.39 | —0.26 |
| $^{R}Q_{2}$ | 1494.28 | 1494.38 | —0.10 | 1463.29 | 1462.90 | +0.39 |
| $^{R}Q_{1}$ | 1478.05 | 1477.93 | +0.12 | 1442.19 | 1442.59 | —0.40 |
| $^{R}Q_{0}$ | 1462.55 | 1462.71 | —0.16 | 1421.07 | 1420.96 | +0.11 |
| $^{P}Q_{1}$ | 1448.38 | 1448.19 | +0.19 | 1398.05 | 1398.52 | —0.47 |
| $^{P}Q_{2}$ | 1434.39 | 1434.06 | +0.33 | 1374.89 | 1375.59 | —0.70 |
| $^{P}Q_{3}$ | 1420.38 | 1420.14 | +0.24 | 1352.40 | 1352.36 | +0.04 |
| $^{P}Q_{4}$ | 1406.36 | 1406.32 | +0.04 | 1329.30 | 1328.92 | +0.38 |
| $^{P}Q_{5}$ | 1392.80 | 1392.54 | +0.26 | 1305.50 | 1305.33 | +0.17 |
| $^{P}Q_{6}$ | — | 1378.76 | — | — | | |
| $^{P}Q_{7}$ | — | 1364.96 | — | — | | |
| $^{P}Q_{8}$ | 1350.79 | 1351.13 | —0.34 | — | | |
| $^{P}Q_{9}$ | 1337.02 | 1337.26 | —0.24 | — | | |
| $^{P}Q_{10}$ | 1323.31 | 1323.33 | —0.02 | — | | |
| $^{P}Q_{11}$ | 1309.17 | 1309.35 | —0.18 | — | | |
| $^{P}Q_{12}$ | 1295.50 | 1295.30 | +0.20 | — | | |
| $^{P}Q_{13}$ | 1281.32 | 1281.19 | +0.13 | — | | |

$\nu_6^0 + A_6(1 - 2\zeta_6^z) - B_6 = 1455.91$ cm$^{-1}$
$A_6(1 - \zeta_6^z) - B_6 = 6.521$ cm$^{-1}$
$(A_6 - A_0) - (B_6 - B_0) = -0.039$ cm$^{-1}$
$\nu_{78} + A_{78}(1 - 2\zeta_{\mathrm{eff}}^z) - B_{78} = 1427.75$ cm$^{-1}$
$A_{78}(1 - \zeta_{\mathrm{eff}}^z) - B_{78} = 11.931$ cm$^{-1}$
$(A_{78} - A_0) - (B_{78} - B_0) = -0.0119$ cm$^{-1}$

Assuming $A_0 = 5.280$ cm$^{-1}$ and $B_0 = B_6 = B_{78} = 0.2992$ cm$^{-1}$ as before, we resolved the above equations to obtain the following parameters

$\nu_6^0 = 1447.85$ cm$^{-1}$   $(\nu_7 + \nu_8)^0 = 1408.86$ cm$^{-1}$
$\alpha_6^A = A_0 - A_6 = 0.039$ cm$^{-1}$   $\alpha_{78}^A = 0.0119$ cm$^{-1}$
$\alpha_6^B = B_0 - B_6 = 0$ (assumed)   $\alpha_{78}^B = 0$ (assumed)
$\zeta_6^z = -0.301 \pm 0.01$   $\zeta_{\mathrm{eff}}^z = -1.316 \pm 0.02$

Comparing these values with those of ref. 15 one realizes that $\nu_6^0$ shows a very small isotopic shift, $\Delta\nu = 0.18$ cm$^{-1}$, as could be expected provided that it is essentially a $\delta(CH_3)$ vibration. On the other hand, $(\nu_7 + \nu_8)^0$ exhibits a larger shift, $\Delta\nu = 1.34$ cm$^{-1}$, due to the presence of the $^{15}$N-sensitive $\nu_8$ fundamental in the combination. According to this, $\zeta_6^z$ should be similar to that in $CH_3CN$ but $\zeta_{\mathrm{eff},\,78}^z$ should have different values (−0.393 and −1.270 respectively). The observed value for $\zeta_{\mathrm{eff},\,78}^z$ differs slightly from the calculated one $((\zeta_7^z + \zeta_8^z) = -1.264)$ due to the uncertainty in $\zeta_8^z$ which has not been experimentally determined but only estimated from the $\zeta$-sum rule.

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