

# INFRARED ABSORPTION SPECTRUM OF SODIUM CITRATE

BY B. R. LAKSHMANAN

(*Department of Physics, Indian Institute of Science, Bangalore-3*)

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## ABSTRACT

The infrared absorption spectrum of sodium citrate has been examined for the first time. The substance has been examined in the state of powder, the region of study being 2–15  $\mu$ . The recorded bands have been correlated with the internal frequencies of the citrate ion and those due to water of crystallisation.

## INTRODUCTION

Little attention appears to have been paid to the infrared study of citrates in general. Raman data on a single crystal of sodium citrate has been recently reported from this laboratory (Krishnan, 1954). This paper presents a preliminary survey of the infrared spectrum of this compound and attempts an assignment of the observed frequencies. Work on citric acid and potassium citrate will be reported later.

## 2. EXPERIMENTAL DETAILS

Sodium citrate was ground to a fine powder and a paraffin oil mull of the same was made. A Perkin Elmer Model 112 Infrared spectrometer with NaCl optics was used to record the spectra. Atmospheric water vapour and carbon dioxide and  $\text{NH}_3$  served as calibration points. The spectral slit-width employed was approximately as follows: 5,000–2,000  $\text{cm}^{-1}$ , 25  $\text{cm}^{-1}$ ; 2,000–1300  $\text{cm}^{-1}$ , 5  $\text{cm}^{-1}$ , 1,300–800  $\text{cm}^{-1}$ , 3  $\text{cm}^{-1}$ ; 800–600  $\text{cm}^{-1}$ , 5  $\text{cm}^{-1}$ . The true per cent. transmission curve was drawn from a point by point division of the records obtained with pure paraffin oil and with the mulled sample.

## 3. RESULTS

Table I contains the observed infrared frequencies along with the Raman frequencies reported by Krishnan (1954). The figures given in the brackets indicate relative intensities of the different frequencies and are based on the per cent. transmission at those frequencies.

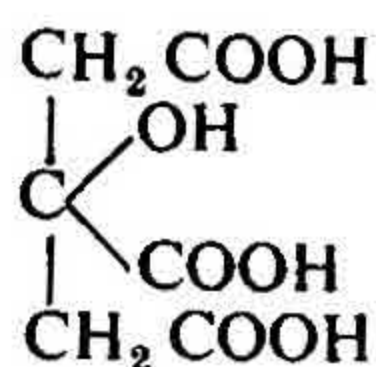
TABLE I

*Infrared and Raman Frequencies (in cm.<sup>-1</sup>)*

Infrared	Raman
	60 (7)
	93 (1)
	111 (1)
	139 (2)
	187 (3)
	233 (5)
	405 (1)
715 (7)	
838 (6)	842 (2)
892 (5)	898 (5)
920 (6)	
938 (5)	945 (5)
963 (4)	968 (4)
1066 (6)	1069 (1)
1078 (7)	1084 (2)
1111 (5)	
1138 (6)	1140 (2)
1174 (5)	
1202 (6)	1206 (4)
1264 (7)	1267 (5)
1298 (5)	1299 (2)
1322 (5)	
1340 (6)	
1379 (9)	
1466 (10)	1436 (6)
	1476 (5)
1544 (6) •	1589 (1)
1628	1625 (1)
2755 (4)	
2880 (10)	2920 (6)
2945 (10)	2935 (8)
	2961 (7)
3241 (5)	
3436 (5)	3435 (4)
3655 (5)	3511 (2)
	3550 (1)
4694 (2)	

## 4. DISCUSSION

Sodium citrate has the chemical formula  $\text{Na}_3\text{C}_6\text{H}_5\text{O}_7 \cdot 5\text{H}_2\text{O}$  and is derived from citric acid,



The bands recorded above can be interpreted in terms of the internal frequencies of the citrate ion and those of the water of crystallisation.

The intense lines at  $2,880$  and  $2,945 \text{ cm.}^{-1}$  are to be attributed to the out of phase and in phase  $\text{CH}_2$  stretching vibrations. The corresponding deformation mode is to be found in the region  $1,320\text{--}1,380 \text{ cm.}^{-1}$ . The bands at  $1,466$  and  $1,544 \text{ cm.}^{-1}$  are due to the antisymmetric and symmetric oscillations of the carboxylate ion. The deformation vibration of this group manifests itself as two medium bands at  $838$  and  $892 \text{ cm.}^{-1}$  while the possible overtones of these bands are to be traced at  $4,674$  and  $2,755$  (Lakshmanan, 1956).

The bands between  $1,300$  and  $1,070 \text{ cm.}^{-1}$  have to be ascribed to the oscillations of the  $\text{C—OH}$  group (West *et al.*, 1956; Padmanabhan, 1948). The bands  $920$ ,  $938$  and  $963$  are possibly due to  $\text{C—C}$  stretching vibrations.

The water of crystallisation yields bands at  $3,650$ ,  $3,436$ ,  $3,241$  and  $1,625 \text{ cm.}^{-1}$ , first three arising out of the  $\text{O—H}$  stretching and the last out of the  $\text{O—H—O}$  bending modes (West *et al.*, 1956).

The crystal structure of sodium citrate has not been worked out so far. X-ray investigations of Burns and Iball (1954) place its symmetry between  $\text{C}_{2v}$  and  $\text{D}_{2d}$ . The remarkable coincidence between Raman and infrared frequency values (*vide* Table I) would appear to favour the former.

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## REFERENCES

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| 1. Krishnan           | .. <i>J. Ind. Inst. Sci.</i> , 1954, 37, 101.  |
| 2. Lakshmanan         | .. <i>Ibid.</i> , 1956, 38.  |
| 3. West <i>et al.</i> | .. <i>Chemical Applications of Spectroscopy</i> (Interscience Publishers, Inc., New York), 1956. |
| 4. Padmanabhan        | .. <i>Proc. Ind. Acad. Sci.</i> , 1948, 28, 494.   |
| 5. Burns and Iball    | .. <i>Acta. Cryst.</i> , 1954, 7, 137.   |