

INFRA-RED ABSORPTION SPECTRA OF COPPER ACETATE, COPPER PROPIONATE AND COPPER BUTYRATE

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ABSTRACT

The infra-red absorption spectra of copper acetate, copper propionate and copper butyrate have been examined in the form of powders in the region 2-15 μ . Tentative assignment of observed infra-red bands to specific molecular groups in these substances has been made.

1. INTRODUCTION

Lecomte and his co-workers (1942) have made an extensive study of the infra-red spectra of salts of organic acids. They confined themselves to the region 600-1600 cm^{-1} and satisfactorily interpreted the observed vibration spectra in that region. The present investigation is concerned with the infra-red absorption spectra of copper acetate, copper propionate and copper butyrate (all having a single water of crystallisation) in a more extended region (600-5000 cm^{-1}). Of these substances copper acetate has been examined by Lecomte in the region 600-1600 cm^{-1} , while the other two have not been studied so far. The results have been compared with the existing data on the infra-red spectra of similar metallic salts and an assignment of the observed frequencies to specific molecular groupings has been attempted.

2. EXPERIMENTAL DETAILS

The substances were examined as powders milled in paraffin oil. A Perkin-Elmer Model 112 single beam double pass infra-red spectrometer with NaCl optics was used to record the spectra. The spectral slit width employed was approximately as follows: 5000-2000 cm^{-1} , 25 cm^{-1} ; 2000-1500 cm^{-1} , 12 cm^{-1} ; 1500-1000 cm^{-1} , 10 cm^{-1} ; 1000-600 cm^{-1} , 4 cm^{-1} . The true percentage transmission curves were drawn from a point by point division of the records obtained with pure paraffin oil and with the milled sample.

3. RESULTS

The percentage transmission curves for copper acetate, copper propionate and copper butyrate are not reproduced here. Table I contains the infra-red data for these compounds as deduced from the absorption curves. The figures given in brackets indicate the relative intensities of the different frequencies and are based on the per cent. transmission at those frequencies.

TABLE I

Infra-red absorption frequencies (cm.⁻¹)

Copper acetate	Copper propionate	Copper butyrate
4774 (4)	4726 (5)	4697 (4)
3441 (10)	3467 (4)	3420 (8)
2937 (10)	2912 (10)	2901 (10)
2759 (3)	2753 (5)	2746 (3)
2493 (3)
1599 (10)	1589 (10)	1596 (10)
..	1453 (10)	1449 (10)
1438 (10)
..	1420 (10)	1426 (10)
..	1377 (10)	1376 (9)
..	..	1347 (8)
..	1305 (9)	1319 (9)
1265 (7)	1246 (7)	1269 (8)
..	..	1212 (6)
1165 (6)	1155 (5)	1165 (6)
1118 (6)	1112 (4)	1102 (7)
1054 (9)	1077 (8)	1053 (4)
1036 (9)	1015 (5)	..
982 (5)	972 (4)	958 (3)
944 (5)	..	933 (3)
..	892 (4)	896 (5)
847 (4)	847 (4)	847 (4)
809 (4)	814 (7)	802 (7)
..	755 (4)	753 (6)
..	711 (5)	724 (6)
666 (10)	677 (6)	662 (8)

4. DISCUSSION

All the three materials show intense bands near 2920 cm.^{-1} which are to be traced to the hydrogen stretching vibrations. Owing to overlapping of these vibrations with those of paraffin oil and owing to poor resolution of NaCl in this region, it is not easy to separate out the C-H vibrations of CH_2 and CH_3 groups. The C-H deformation oscillations give three frequencies (1376, 1346 and 1319) for the butyrate and two (1377 and 1305) for the propionate. The bands in this region are missing in copper acetate and in a number of other acetates examined elsewhere (Duval *et al.*, 1942). This leads one to attribute the frequencies mentioned above to the group C-(CH_2)_n (*cf.* Bellamy, 1954).

One observes two strong bands near 1600 and 1420 cm.^{-1} . These have to be assigned to the symmetric and antisymmetric oscillations of the carboxylate ion. The possible overtones of these bands are found at about 4700 and 2760 cm.^{-1} . It is an established observation (Bellamy, 1954) that, in salts of many organic acids, the strong carbonyl frequency (1730 cm.^{-1}), commonly found in the acids and their esters, vanishes and is replaced by two bands, one between 1610 and 1550 cm.^{-1} and another in the region 1300 - 1420 cm.^{-1} . When ionisation occurs, resulting in the COO^- group, resonance is possible between the two C-O bonds with the consequent disappearance of the C=O bands.

The bands 1265 and 1165 cm.^{-1} (copper acetate), 1246 and 1155 (copper propionate), and 1269 , 1213 , 1165 cm.^{-1} (copper butyrate) can be attributed to the C-O stretching vibrations (*Reference* 3, 4, 5). The bands between 900 and 1000 cm.^{-1} are probably due to the C-C stretching modes. Following Duval *et al.* (1942), one can assign the frequencies in the region 800 - 900 cm.^{-1} to the symmetrical deformation vibration of the COO group. The bands between 700 and 800 cm.^{-1} and the one at 670 are due to the mutual oscillations of the carboxyl and alkyl groups. 3440 cm.^{-1} arises from the water of crystallisation (West *et al.*, 1956).

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