

IR Spectral study of complexation of carboxylic acids with chromium containing complex

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Abstract: Different carboxylic acid were treated with di-tertiary butyl chromate (TBC) a chromium complex in different molar ratio of substrate and reagent. The complexes thus obtained were collected for analysis. During IR spectral analysis different peak were observed. On the basis of peaks observed in IR spectra different functional groups present in the complexes were identified and explained in this research paper.

(Keywords : IR (Infrared) spectroscopy, TBC (Di-tertiarybutylchromate), Caproic acid, Adipic acid)

Introduction

Strong oxidants of chromium(vi) have been used to oxidise several organic as well as inorganic compounds for the very long period. Such chromium(vi) containing oxidants have been used in both media- aqueous medium and non aqueous medium. T.B.C. is the most effective non aqueous oxidant which has been used to oxidize several classes of organic compounds by different groups of coworkers. We particularly studied the oxidation of different carboxylic acid using T.B.C. as oxidant. We treated carboxylic acid with a versatile non aqueous oxidant, ditertiary butyl chromate (T.B.C.) by taking different ratio of substrate and oxidant. The various products were obtained, washed, purified and collected as samples. Further the functional groups present in the complexes were identified by IR spectral analysis of the samples.

Experimental⁴⁻⁸:

- a) **CB2:** Caproic acid was oxidized by TBC in molar ratio 1:0.75 (acid:TBC). The complex thus obtained was analysed by IR spectral analysis.
- b) **CB3:** Caproic acid was oxidized by TBC in molar ratio 1:1 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.
- c) **CB3:** Caproic acid was oxidized by TBC in molar ratio 1:1.25 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.
- d) **CB6:** Caproic acid was oxidized by TBC in molar ratio 1:0.5 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.
- e) **AB1:** Adipic acid was oxidized by TBC in molar ratio 1:0.5 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.
- f) **AB2:** Adipic acid was oxidized by TBC in molar ratio 1:0.75 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.
- g) **AB4:** Adipic acid was oxidized by TBC in molar ratio 1:1.25 (acid : TBC). The complex thus obtained was analysed by IR spectral analysis.

Result and discussion¹⁻³:**a) IR spectra of CB2:**

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
771.78	Cr-O (str.)
1069.05	Cr- O (str.)
1155.4	C-O (str.)
1402.94	OH bending or CH_2 bending
1631.5	$\text{C}=\text{O}$ str. -CHO or -COOH
2920.11	C-H (str.) due to -CHO or -COOH
3397.38	OH (str.)

b) IR spectra of CB3:

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
669.05, 770.58, 929.3	Cr-O (str.)
1069.98	C- O (str.)
1215.66	C-O (str.)
1422.79	OH bending or CH_2 bending
1602.4	$\text{C}=\text{O}$ str. -CHO or - COOH
2957.94, 3019.64	C-H (str.) due to -CHO or -COOH
3407.26	OH (str.)

c) IR spectra of CB4

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
669.1, 770.46, 929.7	Cr-O (str.)
1070, 1156.65, 1215.68	C-O (str.)
1416.95	OH bending or CH_2 bending
1631.5	$\text{C}=\text{O}$ str. -CHO or -COOH
2400.2	Chelation due to H bonding
2928.39, 3019.62	C-H (str.) due to - CHO or COOH
3410.03	OH (str.)

d) IR spectra of CB6

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
669.25, 760.3, 929.7	Cr-O (str.)
1069.32, 1156.06, 1215.67	C-O (str.)
1404.29	OH bending or CH_2 bending
1633.71	$\text{C}=\text{O}$ str. -CHO or - COOH
2399.97	Chelation due to H bonding
3019.57	C-H (str.) due to - CHO or COOH
3413.46	OH (str.)

e) IR spectra of AB1:

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
668.97	Cr-O (str.)
757.43	Cr- O (str.)
929.07	Cr- O (str.)
1215.39	C-O (str.)
1398.98	C-OH bending or CH_2 bending
1613.97	α , β unsaturated $\text{C}=\text{O}$ str. or $\text{C}=\text{C}$ COOH
2400.08	chelation
3019.55	C-H (str.)
3413.62	OH (str.)

f) IR spectra of AB2:

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
669.02	Cr-O (str.)
759.07	Cr- O (str.)
1215.47	C-O (str.)
1397.21	C-OH bending or CH_2 bending
1617.97	α , β unsaturated $\text{C}=\text{O}$ str. or $\text{C}=\text{C}$ COOH
3019.51	C-H (str.)
3431.81	OH (str.)

g) IR spectra of AB4

FTIR Peaks (Wave no. cm^{-1})	Group Assignments
669	Cr-O (str.)
768.7	Cr- O (str.)
1068.67	Cr- O (str.)
1215.64	C-O (str.)
1396.57	C-OH bending or CH_2 bending
1615.16	α, β unsaturated C=O str. or C=C COOH
3019.59	C-H (str.)
3424.85	OH (str.)

Conclusion:

The IR spectra of complexes show that all the complexes have Cr-O bond which absorbs in range 586 to 1000 cm^{-1} , most of them have C-O group which absorbs in range 1000 to 1250 cm^{-1} , all the complexes have C=O str. (COO^- , COOH , CHO) which absorbs in range 1300 to 1625 cm^{-1} , complexes absorbs in range 2800 to 3000 cm^{-1} , complexes absorbs in range 3050 to 3700 cm^{-1} which indicate the presence of OH (str.) or polymeric association. Thus the peaks observed by IR spectra help in the determination of structure and formula of complexes.

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