Practical Organic Chemistry

5th Sem
Practical – 1
Paper- C12P

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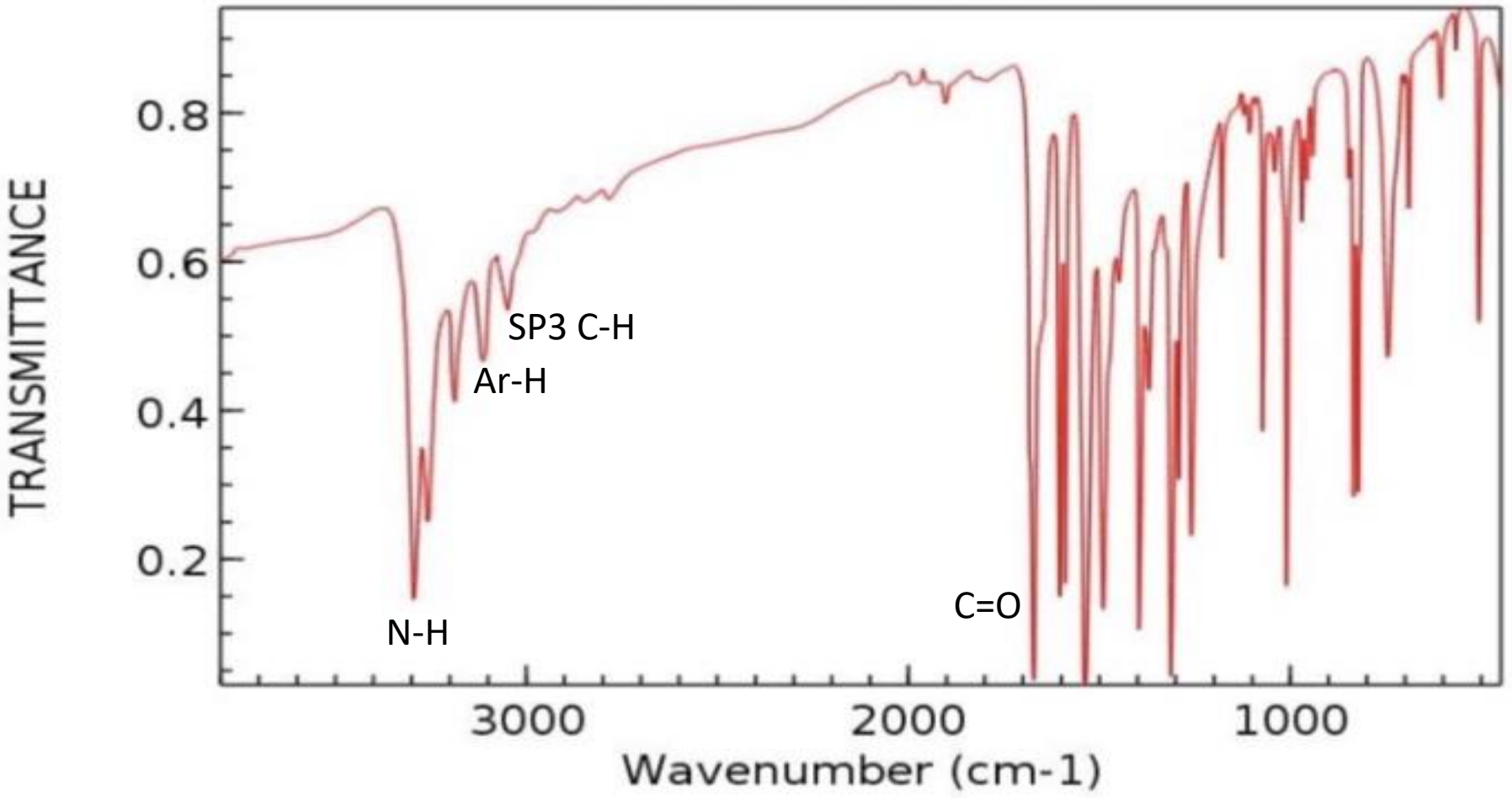
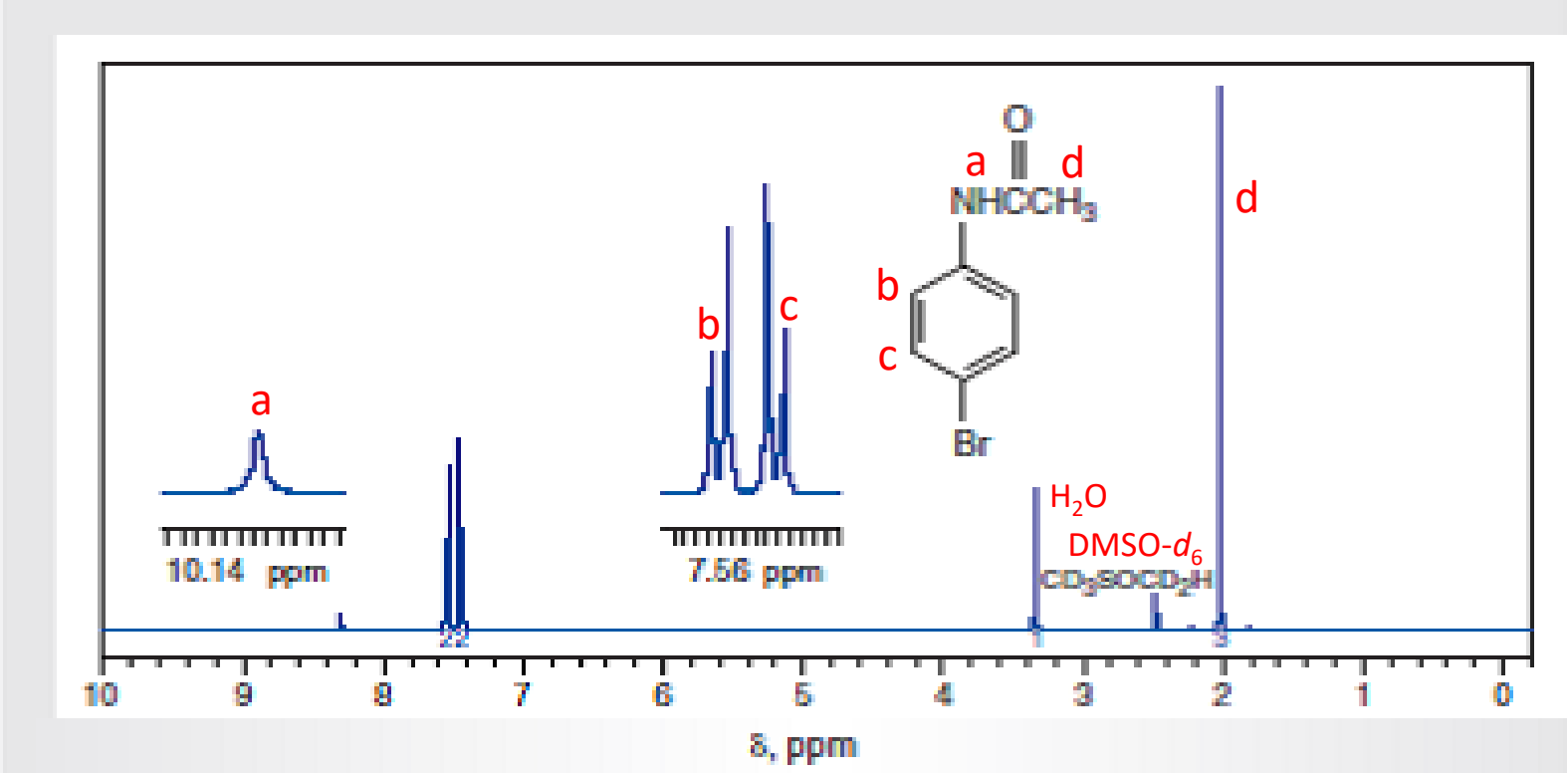
4-Bromoacetanilide: IR spectrum



Wavenumber (cm^{-1})	Intensity	Assignment
3300	Strong	N-H stretching (symmetric and asymmetric)
3100	Medium	Aromatic C-H stretching
3000	Week	Aliphatic C-H stretching
1690	Strong	C=O stretching
1540	Strong	N-H bending

4-Bromoacetanilide: ^{1}H NMR spectra in DMSO-d_6

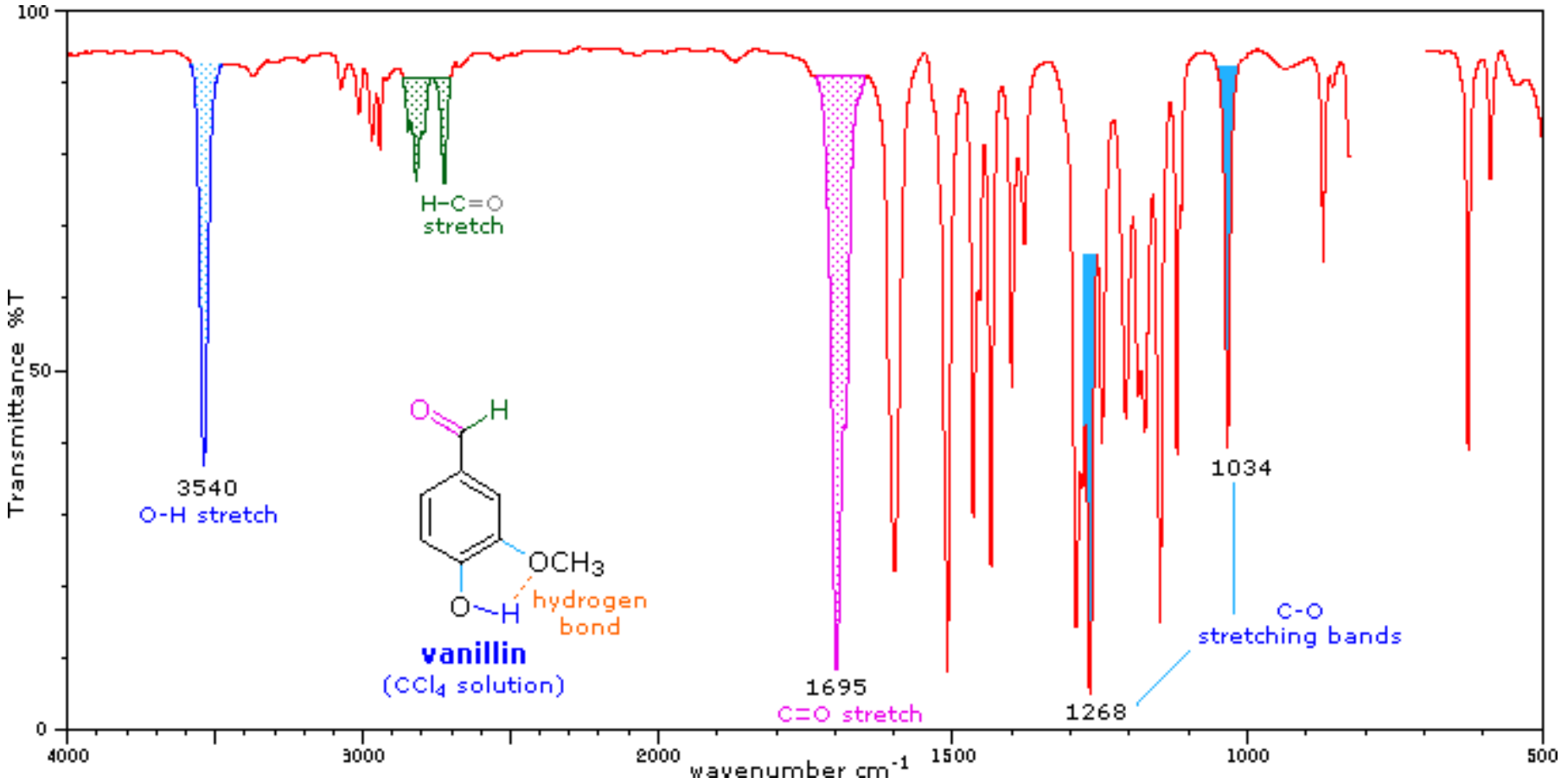


(a) ^{1}H NMR spectrum (300 MHz).
(b) ^{13}C NMR data: δ 25.1, 115.5, 121.9, 132.5, 139.7, 169.5.

The amine proton is in conjugation with the carbonyl group, thus making the N atom partially more electronegative. Hence, b proton comes downfield than c proton.

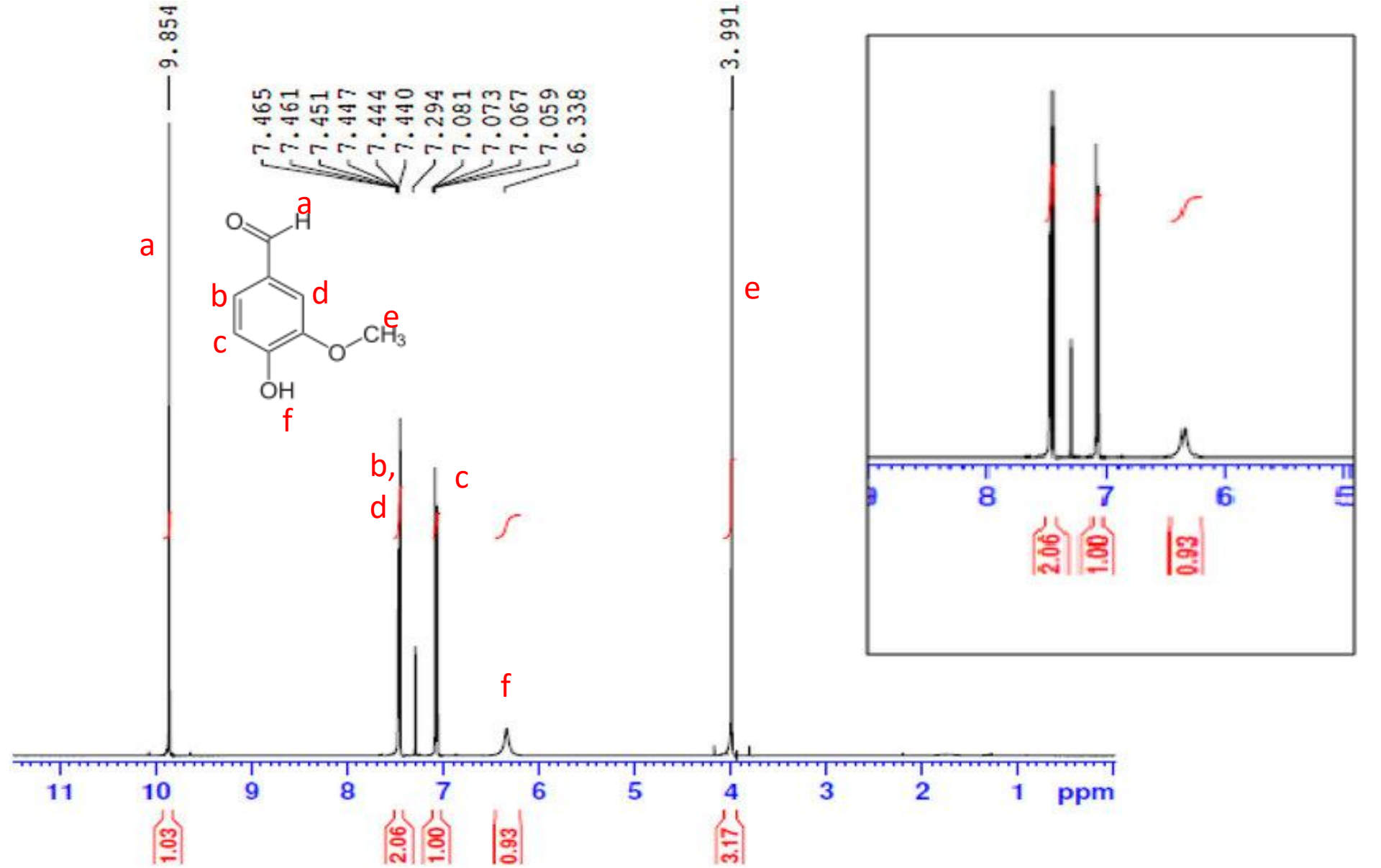
δ ppm	Assigned proton	Integration and multiplicity	Explanation
10.1	a	1 proton, broad singlet	Amine proton, deshielded due to –I effect of –C=O and broad due intermolecular H-bonding
7.56	b	2 proton, doublet	The amine proton is in conjugation with the carbonyl group, thus making the N atom partially more electronegative. Hence, b proton comes downfield than c proton. Doublet due to coupling with c proton
7.45	c	2 proton, doublet	Ortho to the –Br atom. Electronegativity of Br is less than N atom, thus appears upfield. Doublet due to coupling with b proton
2.00	d	3 proton, singlet	-CH3 proton attached with carbonyl group. –I effect of –C=O group Deshields the resonance

Vaniline: IR spectrum



Wavenumber (cm^{-1})	Intensity	Assignment
3540	Strong	O-H stretching
3050-3000	week	Aromatic C-H stretching
2950-2900	Week	Aliphatic C-H stretching
2850-2700	week	Aldehyde C-H stretching
1695	Strong	C=O stretching
1268	Strong	C-O stretching

Vaniline: ^{1}H NMR spectra in $CDCl_3$



δ ppm	Assigned proton	Integration and multiplicity	Explanation
9.8	a	1 proton, singlet	Aldehyde proton, deshielded due to anisotropic and –I effect of –C=O group
7.44-7.46	b, d	2 proton, multiplet	Ortho to the –CHO group and due to -I effect of –CHO it is more downfield. Multiplet as non-symmetric b and d protons merged together.
7.08	c	1 proton, doublet	Ortho to the –OH group and due to +R effect of –OH group it appears upfield. Doublet due to coupling with H_b
6.34	f	1 proton, broad singlet	-OH proton, broad due to intermolecular H-bonding
3.99	e	3 proton, singlet	-CH_3 proton attached with electronegative O atom and deshields the resonance