B.Sc. Semester-VI
Paper CC-XIV
Organic Chemistry-V

III. Nuclear Magnetic Resonance Spectroscopy

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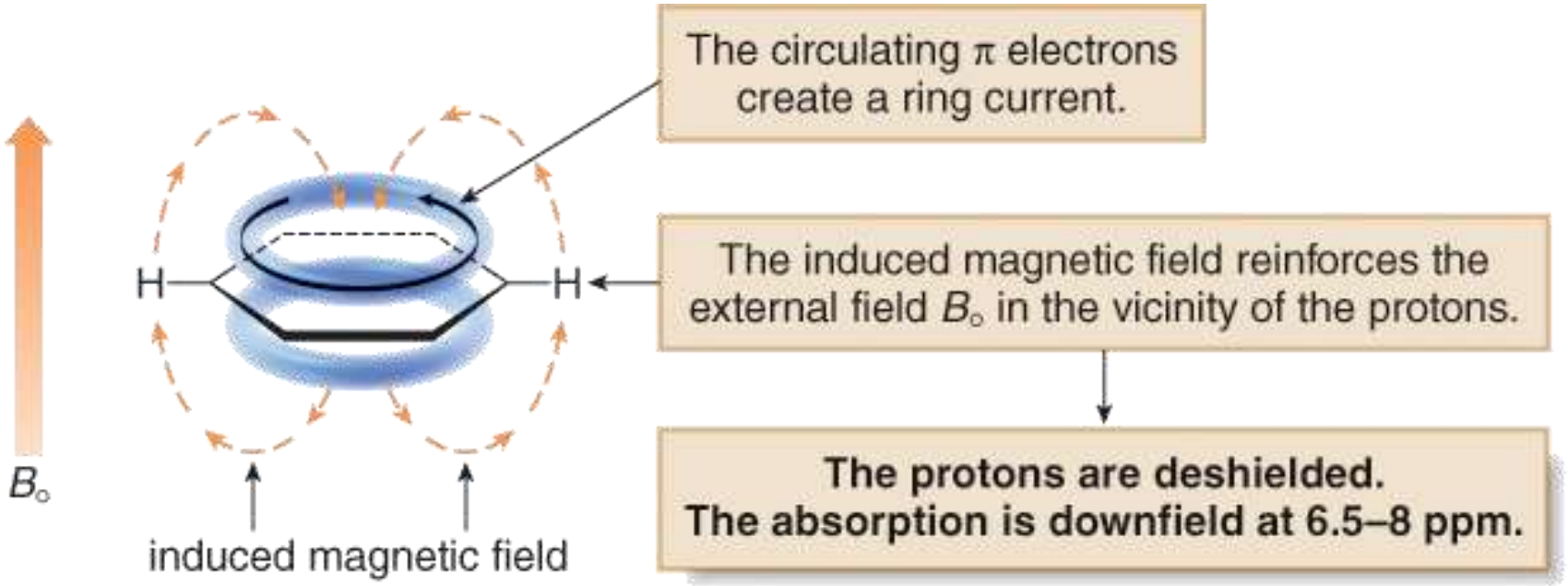
Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR–Chemical Shift Values

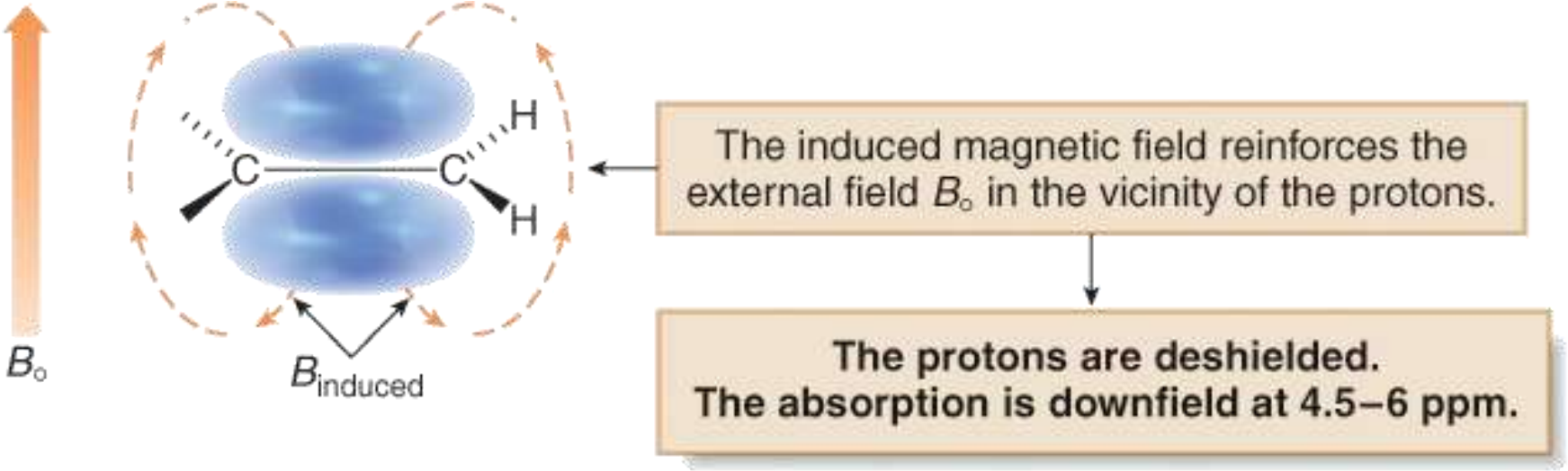
- In a magnetic field, the six π electrons in benzene circulate around the ring creating a ring current.
- The magnetic field induced by these moving electrons reinforces the applied magnetic field in the vicinity of the protons.
- The protons thus feel a stronger magnetic field and a higher frequency is needed for resonance. Thus they are deshielded and absorb downfield.



Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR—Chemical Shift Values

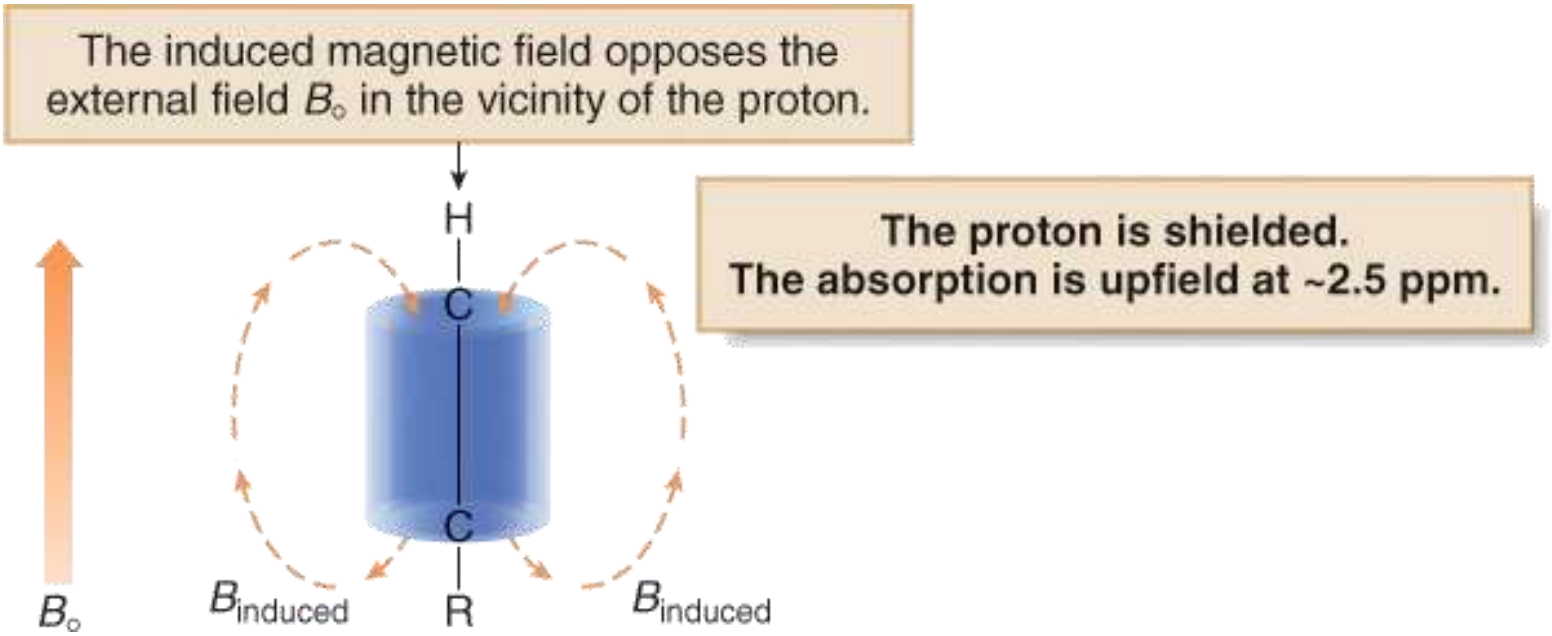
- In a magnetic field, the loosely held π electrons of the double bond create a magnetic field that reinforces the applied field in the vicinity of the protons.
- The protons now feel a stronger magnetic field, and require a higher frequency for resonance. Thus the protons are deshielded and the absorption is downfield.



Nuclear Magnetic Resonance Spectroscopy

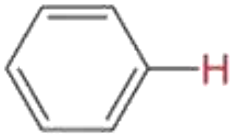
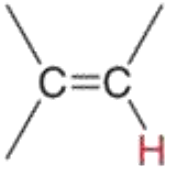
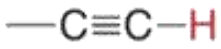
^{1}H NMR—Chemical Shift Values

- In a magnetic field, the π electrons of a carbon-carbon triple bond are induced to circulate, but in this case the induced magnetic field opposes the applied magnetic field (B_0).
- Thus, the proton feels a weaker magnetic field, so a lower frequency is needed for resonance. The nucleus is shielded and the absorption is upfield.



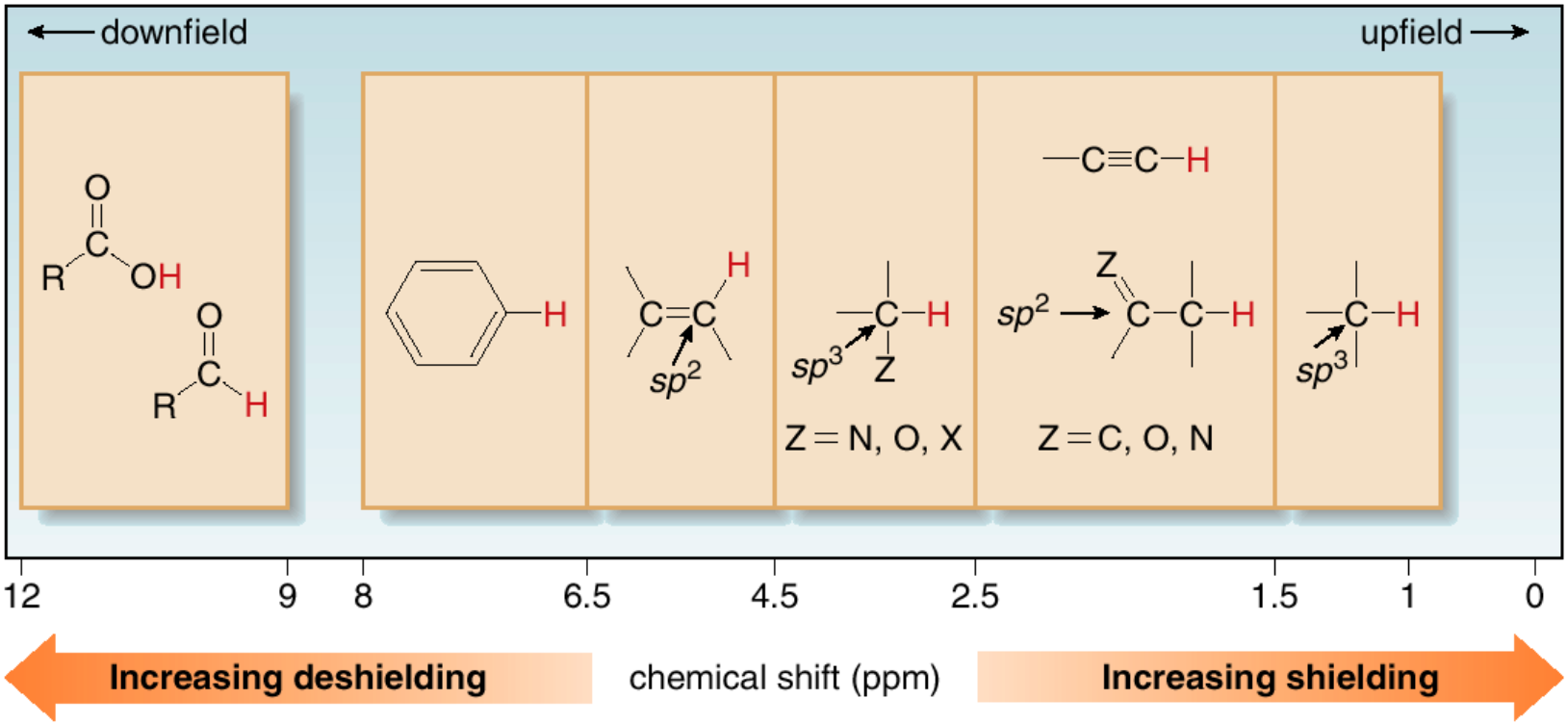
Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR–Chemical Shift Values

Proton type	Effect	Chemical shift (ppm)
	highly deshielded	6.5–8
	deshielded	4.5–6
	shielded	~2.5

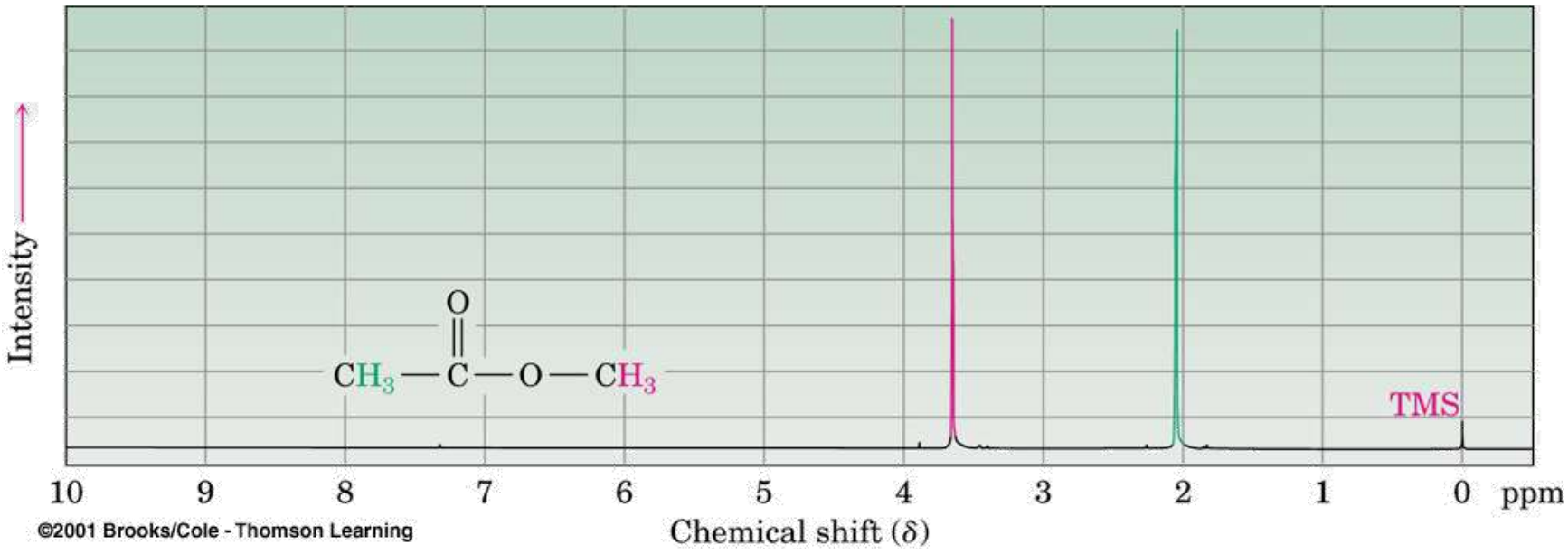
Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR—Chemical Shift Values



- Shielded protons absorb at lower chemical shift (to the right).
- Deshielded protons absorb at higher chemical shift (to the left).

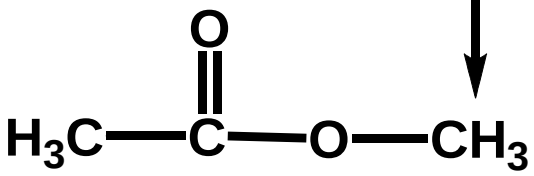
^{1}H NMR of Methyl Acetate



Base Chemical Shift = 0.87 ppm

one α R–C(=O)–O— = 2.88 ppm

TOTAL = 3.75 ppm

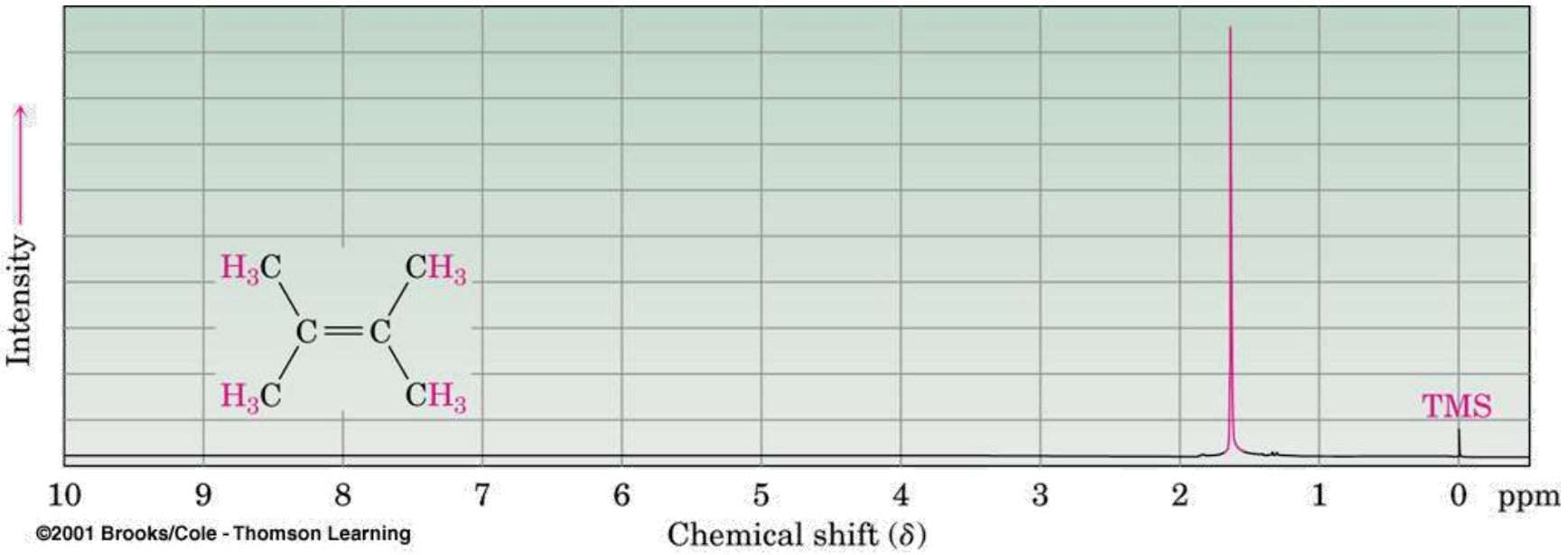


Base Chemical Shift = 0.87 ppm

one α —C(=O)–R = 1.23 ppm

TOTAL = 2.10 ppm

2,3-Dimethyl-2-Butene



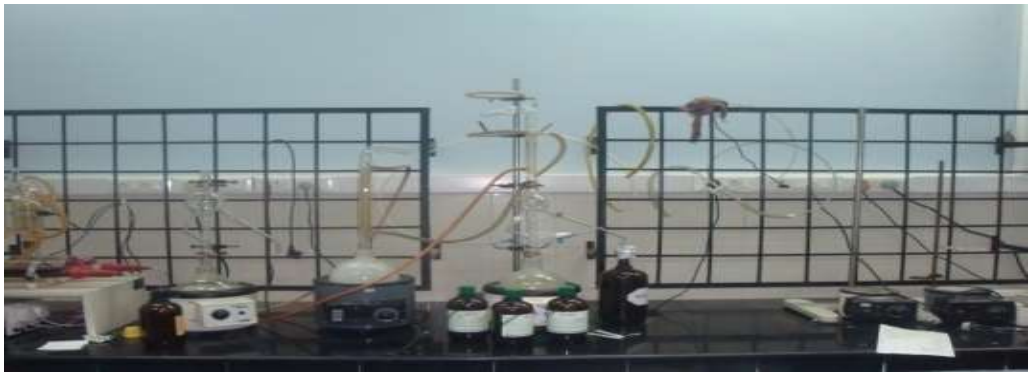
(Hydrogen under consideration)

Base Chemical Shift = 0.87 ppm

one $\alpha_{H_2C=\underset{H}{C}-}$ (CH_3) = 0.78 ppm

TOTAL = 1.65 ppm

Thank You



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