

Infrared (IR) Spectroscopy



Irradiate sample with IR light

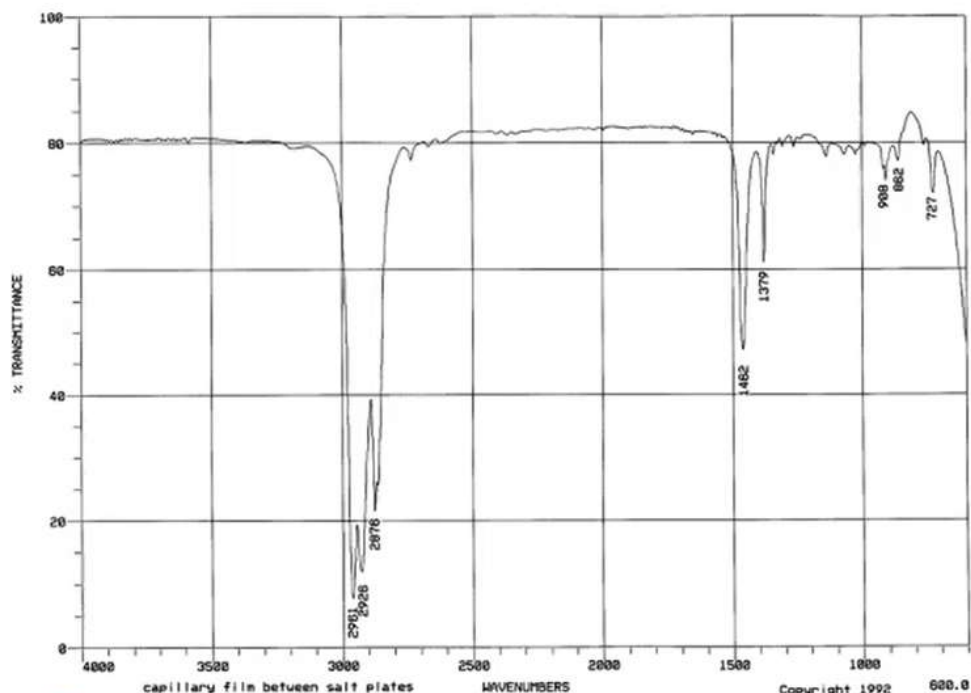
Record frequencies that are absorbed

Certain functional groups have characteristic absorptions

Intensity of absorption is proportional to change in dipole

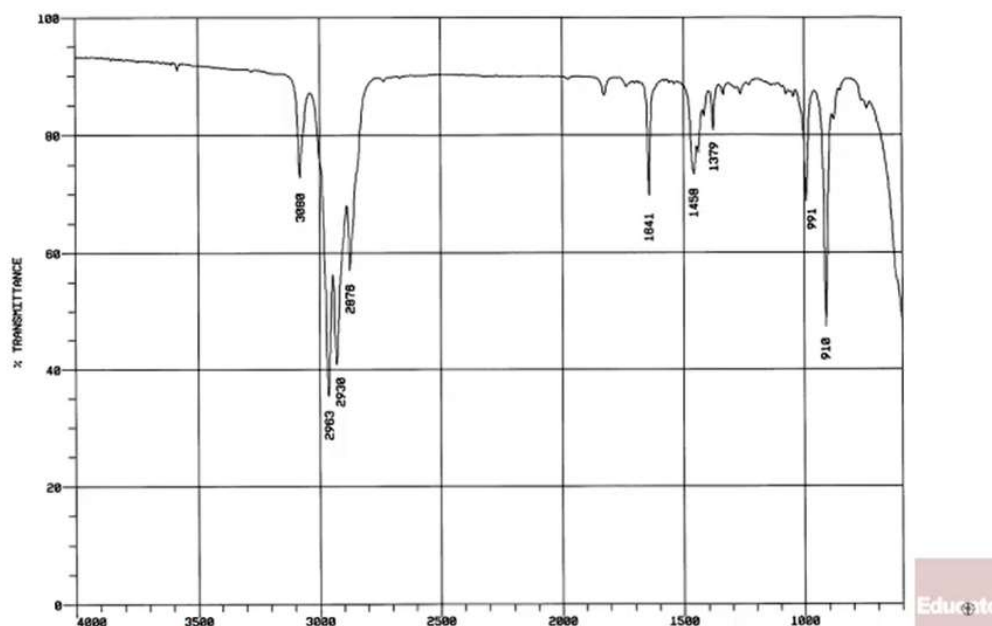
IR Spectrum of an Alkane

Pentane



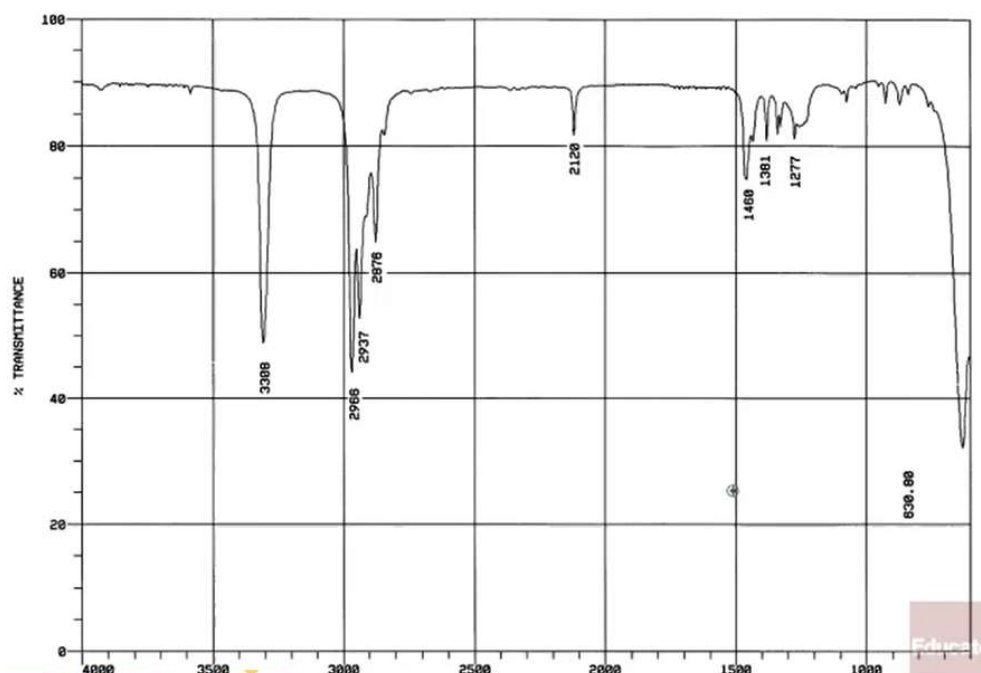
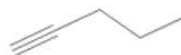
IR Spectrum of an Alkene

1-Pentene



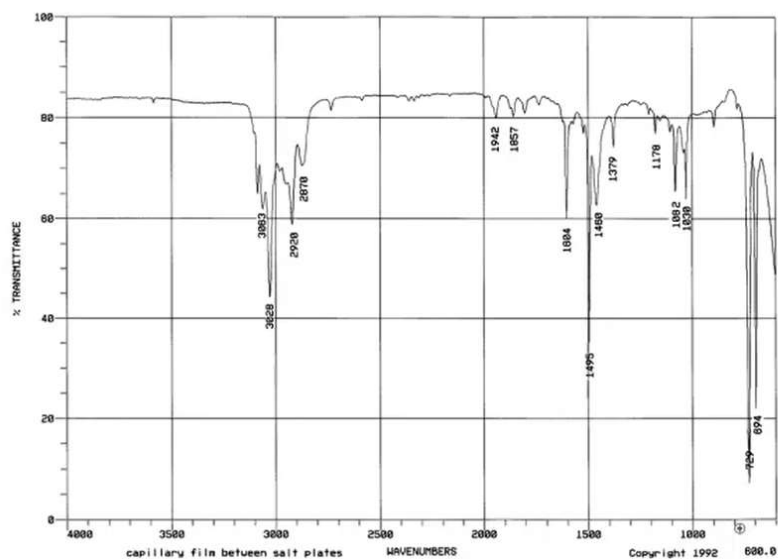
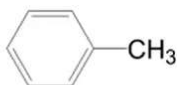
IR Spectrum of an Alkyne

1-Pentyne



IR Spectrum of an Aromatic Compound

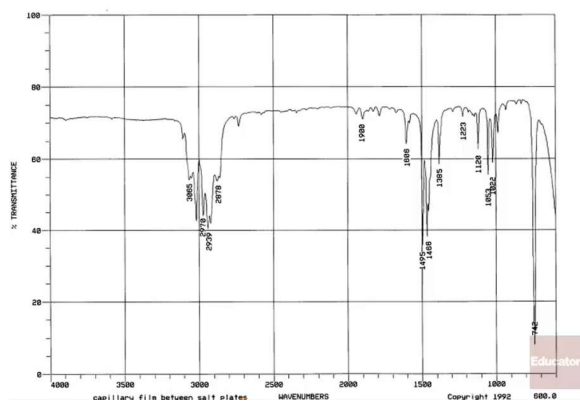
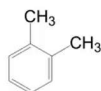
Methylbenzene



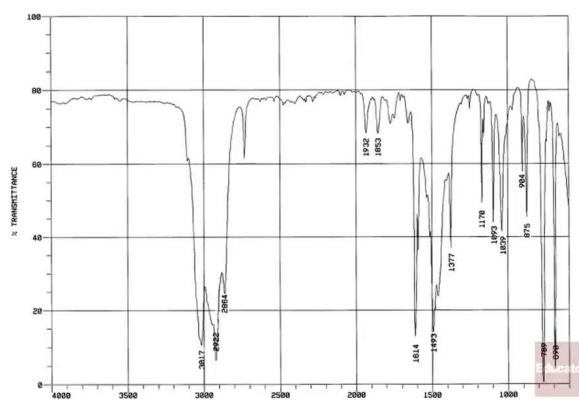
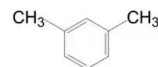
IR of Substituted Aromatic Compounds

Type	Out-of-plane bending peaks (cm ⁻¹)
monosubstituted	~750 and ~690
1,2-disubstituted (ortho)	~750
1,3-disubstituted (meta)	three peaks: ~880, ~750, ~690
1,4-disubstituted (para)	~815

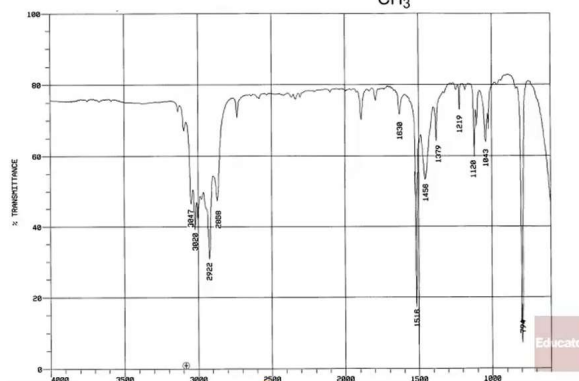
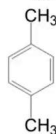
1,2-dimethylbenzene



1,3-dimethylbenzene

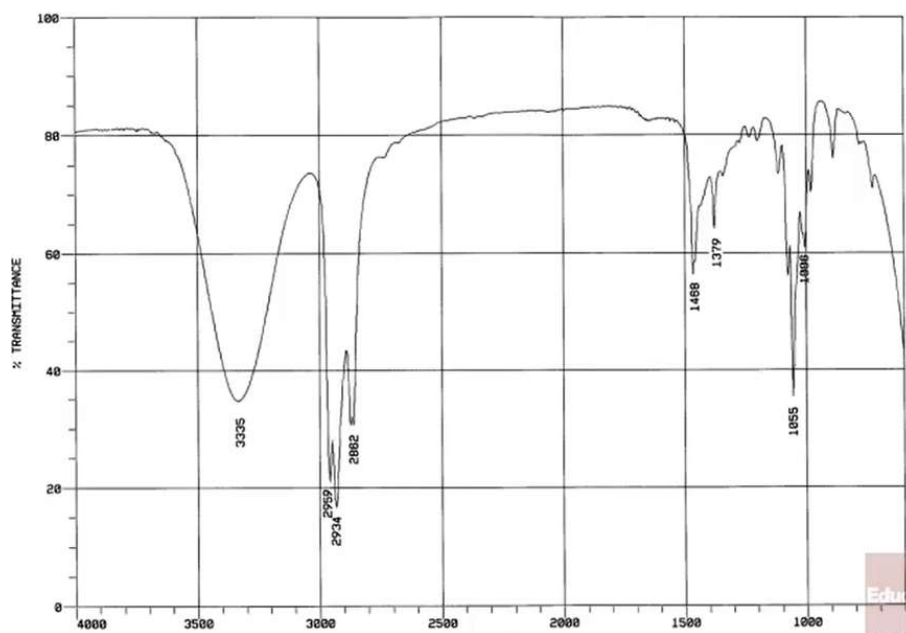


1,4-dimethylbenzene



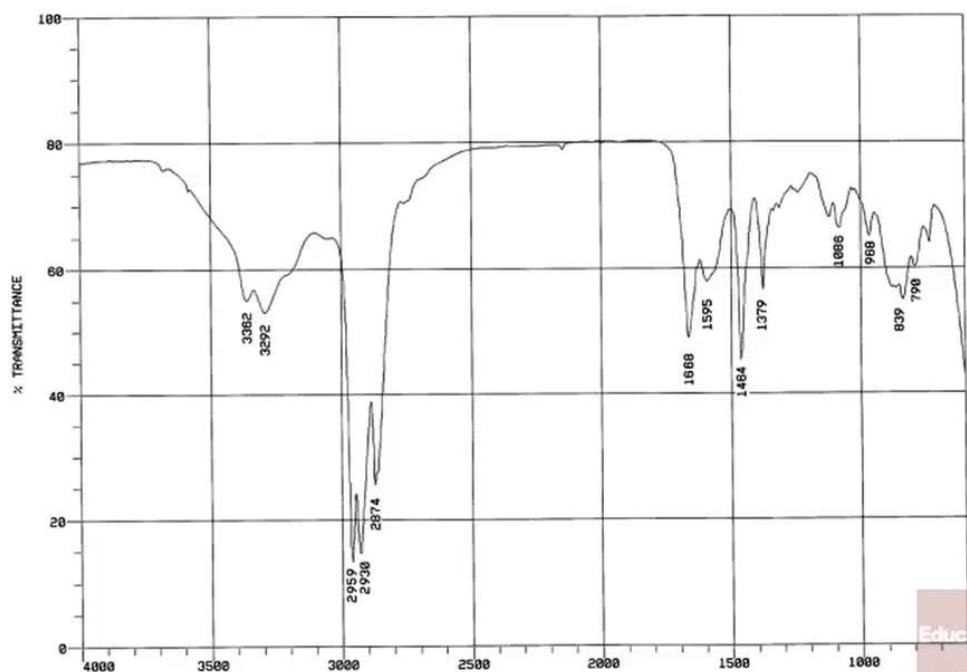
IR Spectrum of an Alcohol

1-pentanol



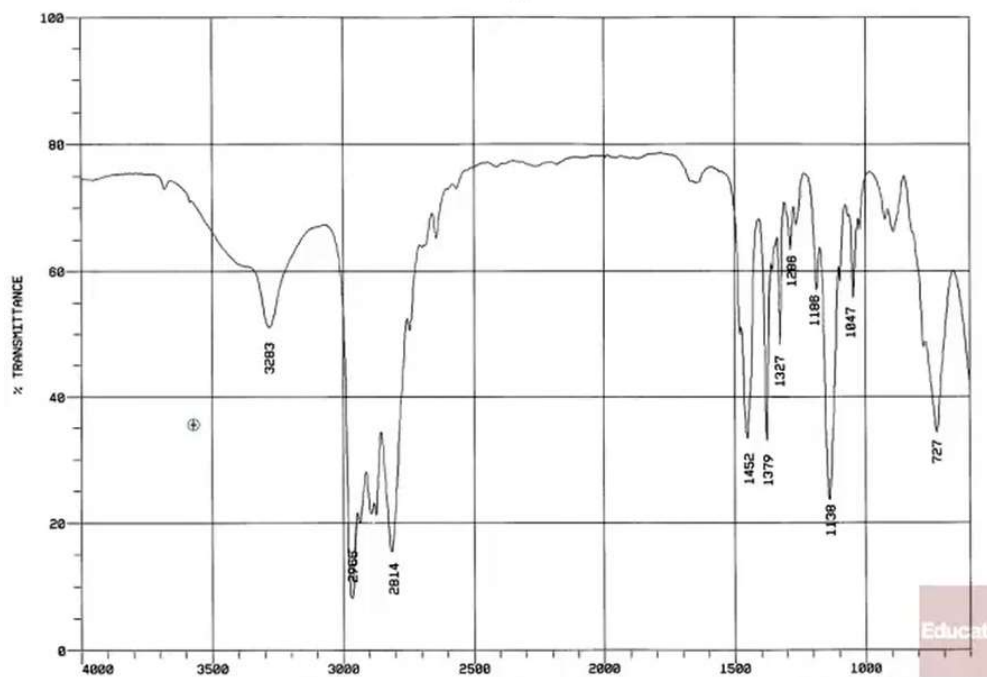
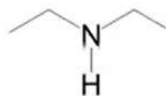
IR Spectrum of an Amine

1-butanamine



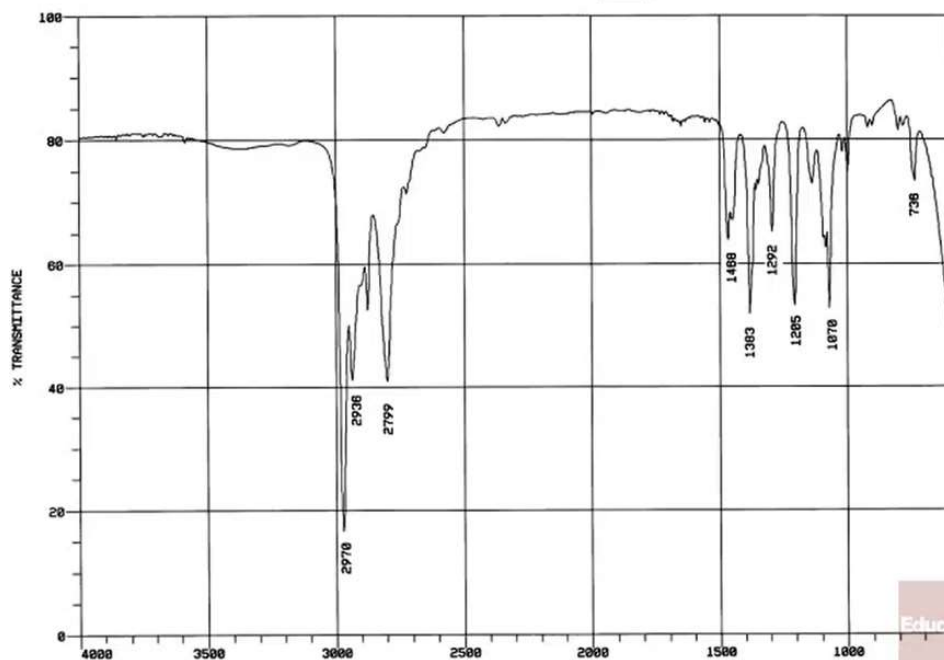
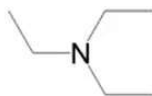
IR Spectrum of a 2° Amine

diethylamine



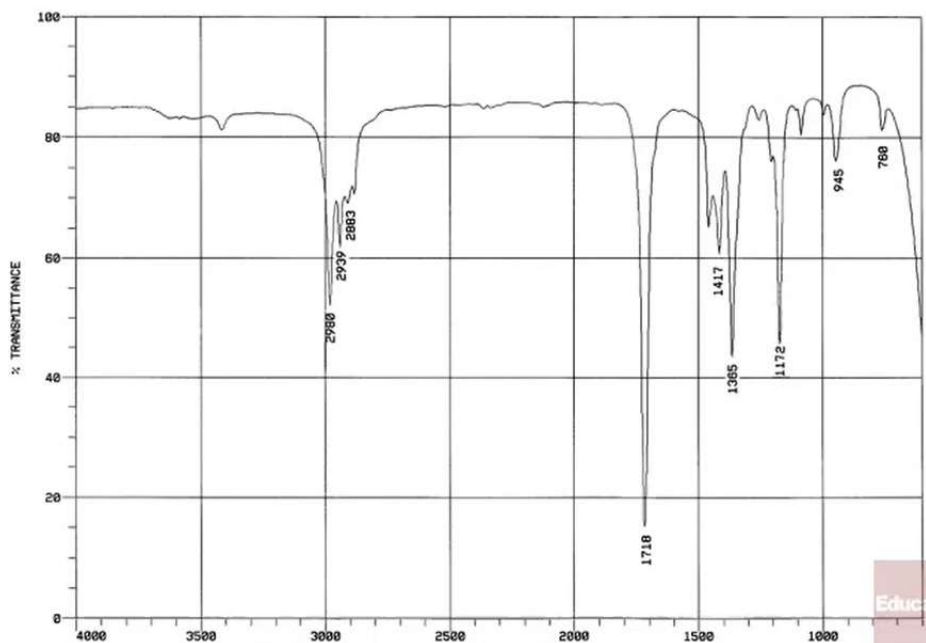
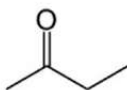
IR Spectrum of a 3° Amine

triethylamine



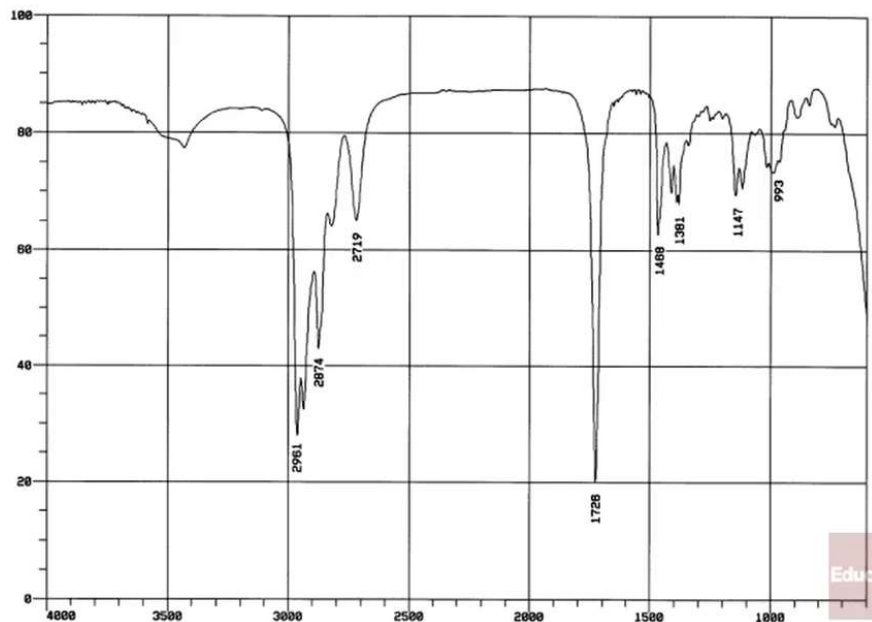
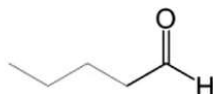
IR Spectrum of a Ketone

2-butanone



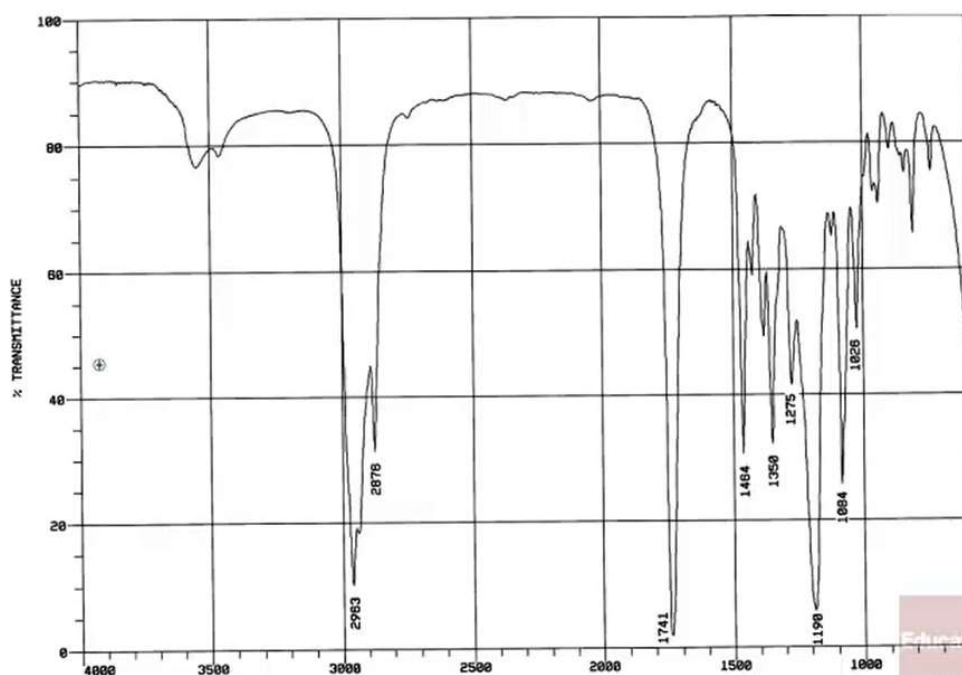
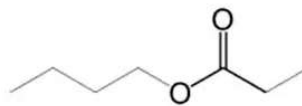
IR Spectrum of an Aldehyde

pentanal



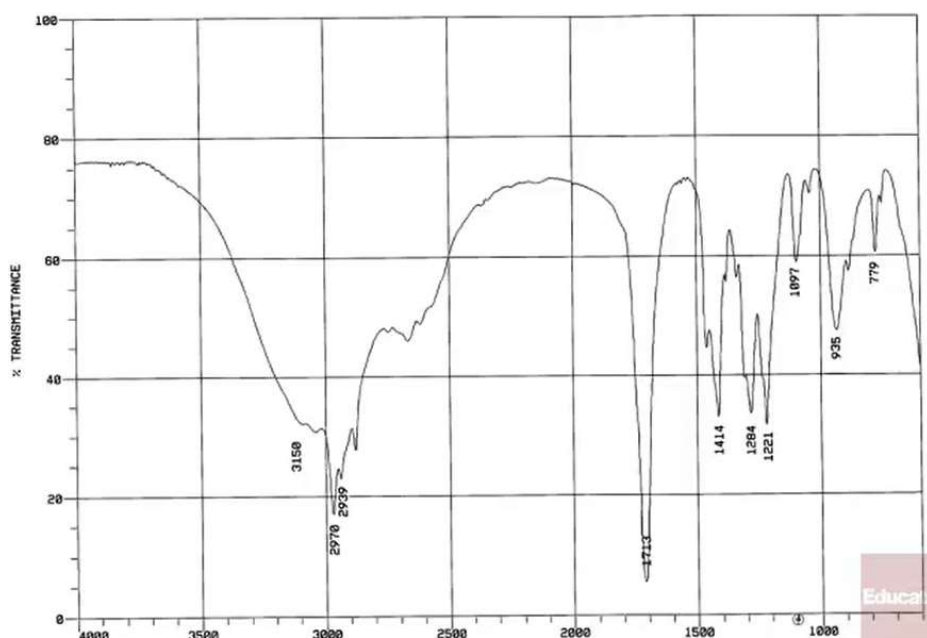
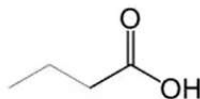
IR Spectrum of an Ester

butyl propanoate



IR Spectrum of a Carboxylic Acid

butanoic acid



Sample IR Correlation Chart

Wavenumber	Functional Group
3600-3300 (s, broad)	O-H stretch (alcohol, phenol)
3400-2400 (s, very broad)	O-H stretch (carboxylic acid)
3500-3300 (m)	N-H stretch
3300 (s)	sp C-H stretch (alkyne $\equiv$ C-H)
3080-3020 (m) (just above 3000)	sp ² C-H stretch (alkene or aromatic =C-H)
2960-2850 (s) (just below 3000)	sp ³ C-H stretch (alkane)
2850 and 2750 (w)	aldehyde C-H stretch (O=C-H)
2260-2100 (w)	C $\equiv$ C stretch (alkyne)
2260-2220 (w)	C $\equiv$ N stretch (nitrile)
1680-1620 (v)	C=C stretch (alkene or aromatic)
1750-1650 (s)	C=O stretch
1300-1000 (s)	C-O stretch (ether, ester)

Educator

Predicting IR Spectra: Sample Structures

Indicate ALL of the significant peaks you would expect to find in the IR spectrum of each compound. (e.g., sp² CH above 3000 or C=O around 1700)

