

Ενόργανη Χημική Ανάλυση (ΜΠ 212)

Καθ. Έλια Ψυλλάκη

Εργαστήριο Υδατικής Χημείας
Σχολή Χημικών Μηχανικών και
Μηχανικών Περιβάλλοντος
Πολυτεχνείο Κρήτης

Γραφείο διδάσκουσας: Κ1.102

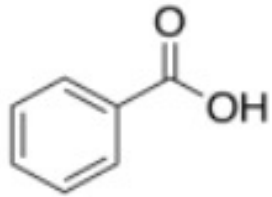
Τηλ: 2821037810

email: epsillakis@tuc.gr

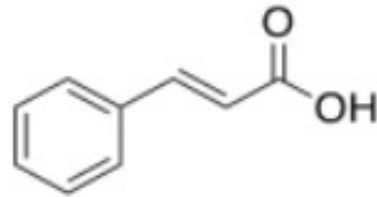
Ασκήσεις UV-Vis Spectra

ΑΣΚΗΣΗ 1

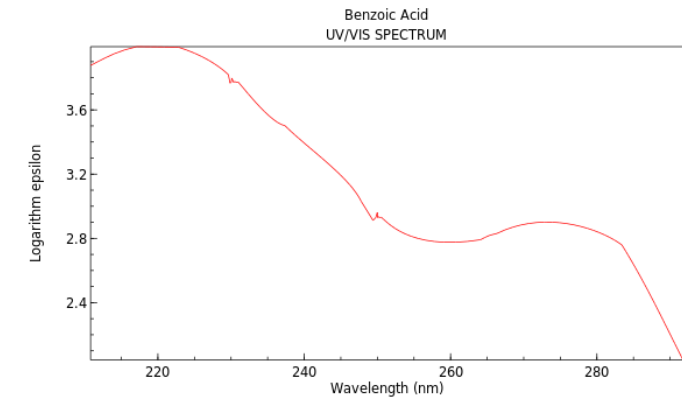
Το βενζοϊκό οξύ έχει μέγιστη απορρόφηση στα 230 nm. Πού περιμένετε να δείτε τη μέγιστη απορρόφηση σε κινναμικό οξύ;



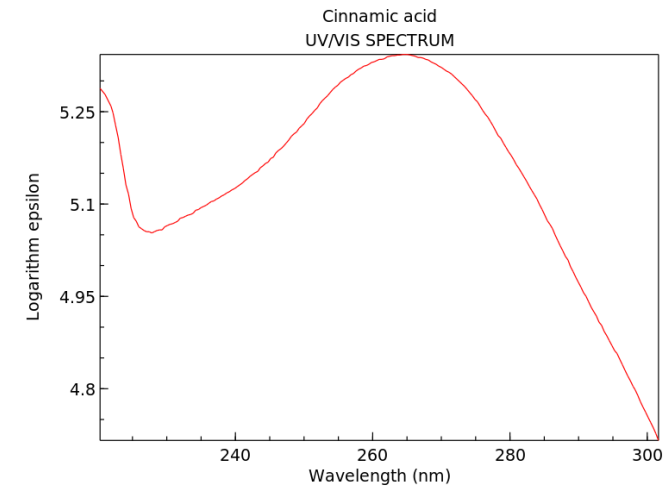
benzoic acid



cinnamic acid



NIST Chemistry WebBook (<https://webbook.nist.gov/chemistry>)



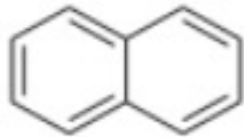
NIST Chemistry WebBook (<https://webbook.nist.gov/chemistry>)

	$\lambda_{\max}$ (nm)
C=C	170
C=C-C=C	220
C=C-C=C-C=C	260

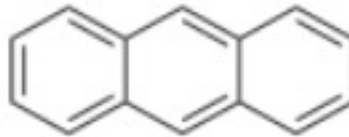
Λύση: 270-280 nm

ΑΣΚΗΣΗ 2

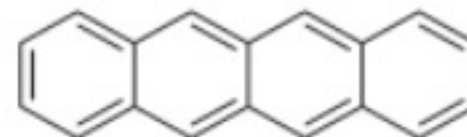
Τα πολυαρωματικά συστήματα έχουν μάλλον περίπλοκα φάσματα υπεριώδους ακτινοβολίας, αλλά καθώς προστίθεται κάθε επιπλέον αρωματικός δακτύλιος, εμφανίζεται μια μετατόπιση περίπου 30 nm στο μέγιστο απορρόφησης της πιο εμφανούς κορυφής. Εάν η ναφθαλίνη έχει $\lambda_{\max}$ στα 220 nm, πού θα βλέπατε τη $\lambda_{\max}$ για το ανθρακένιο και το τετρακενίο;



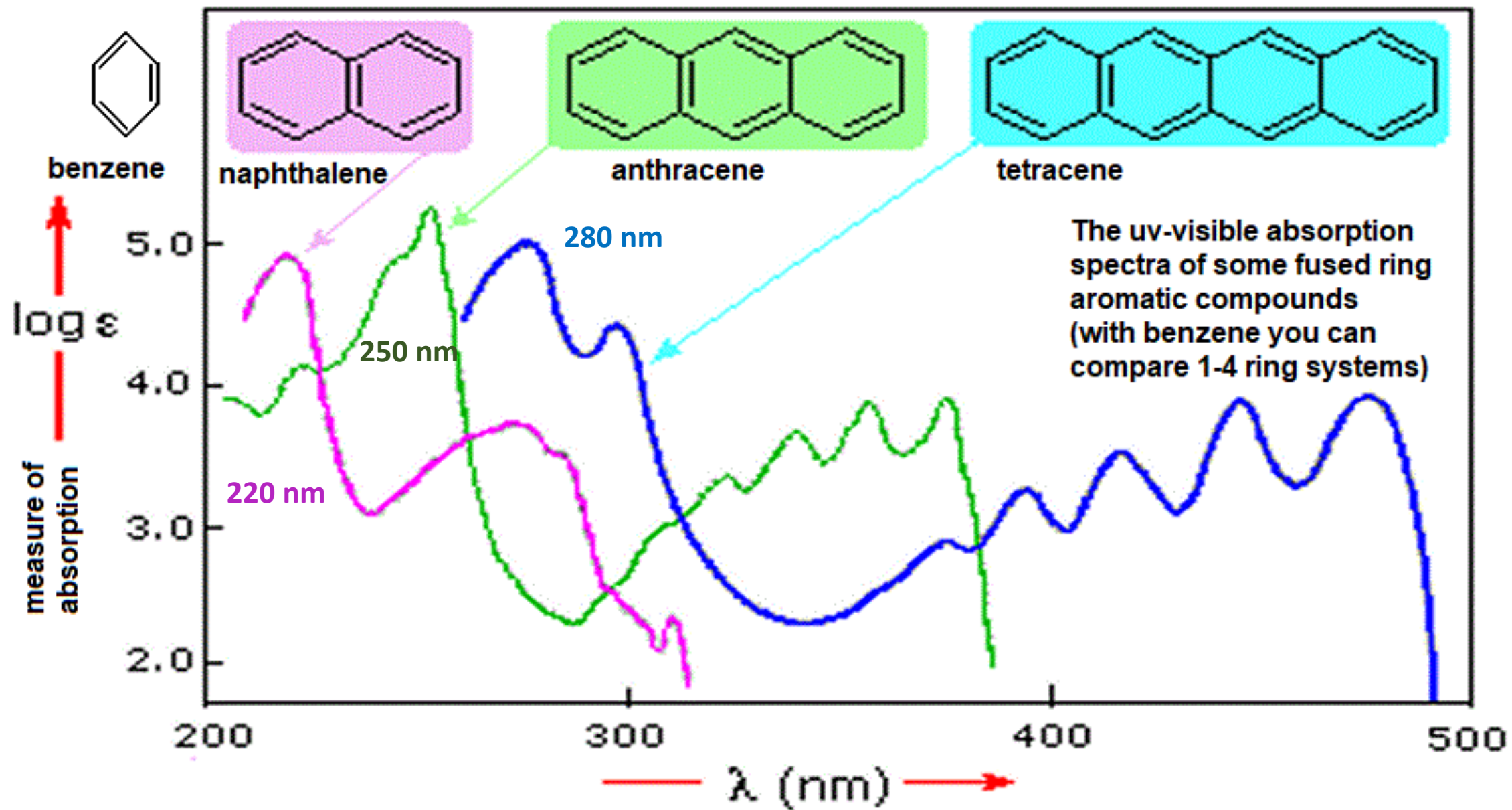
naphthalene



anthracene

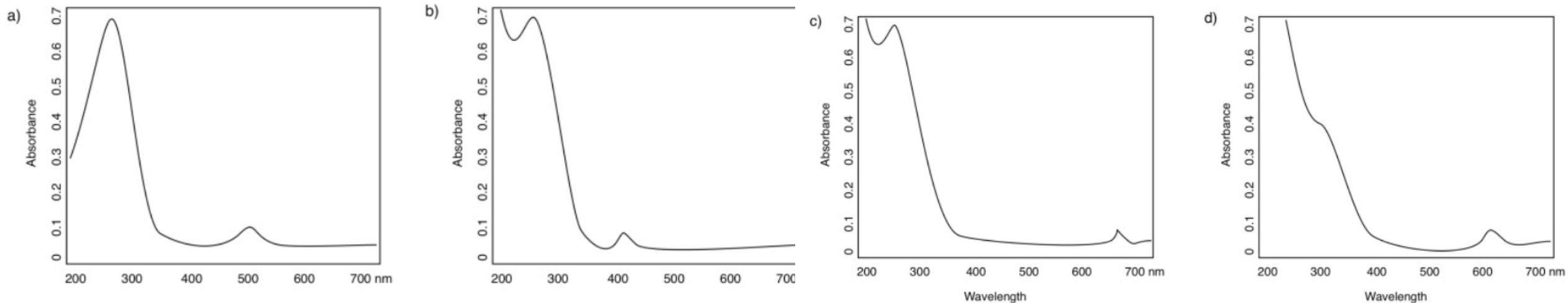


tetracene



ΑΣΚΗΣΗ 3

Βρείτε το χρώμα των παρακάτω ενώσεων

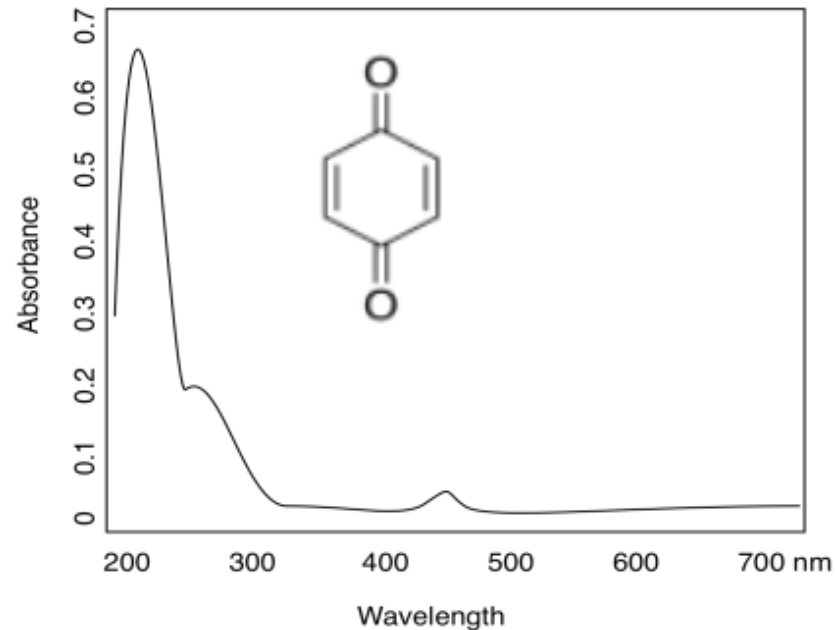


ΠΙΝΑΚΑΣ 18-1 Χρώματα στο ορατό φως		
Μήκος κύματος μέγιστης απορρόφησης (nm)	Χρώμα που απορροφάται	Χρώμα που παρατηρείται
380-420	Ιώδες	Πράσινο-κίτρινο
420-440	Ιώδες-μπλε	Κίτρινο
440-470	Μπλε	Πορτοκαλί
470-500	Μπλε-πράσινο	Κόκκινο
500-520	Πράσινο	Μωβ-κόκκινο
520-550	Κίτρινο-πράσινο	Ιώδες
550-580	Κίτρινο	Ιώδες-μπλε
580-620	Πορτοκαλί	Μπλε
620-680	Κόκκινο-πορτοκαλί	Μπλε-πράσινο
680-780	Κόκκινο	Πράσινο

ΑΣΚΗΣΗ 4

Οι οργανικές ενώσεις, όπως τα μέταλλα μετάπτωσης, μπορούν να έχουν απορροφήσεις ποικίλης ισχύος. Εξετάστε τον ακόλουθο πίνακα για την κίνηση και σχεδιάστε το UV-VIS φάσμα του. Τι χρώμα είναι αυτή η ένωση?

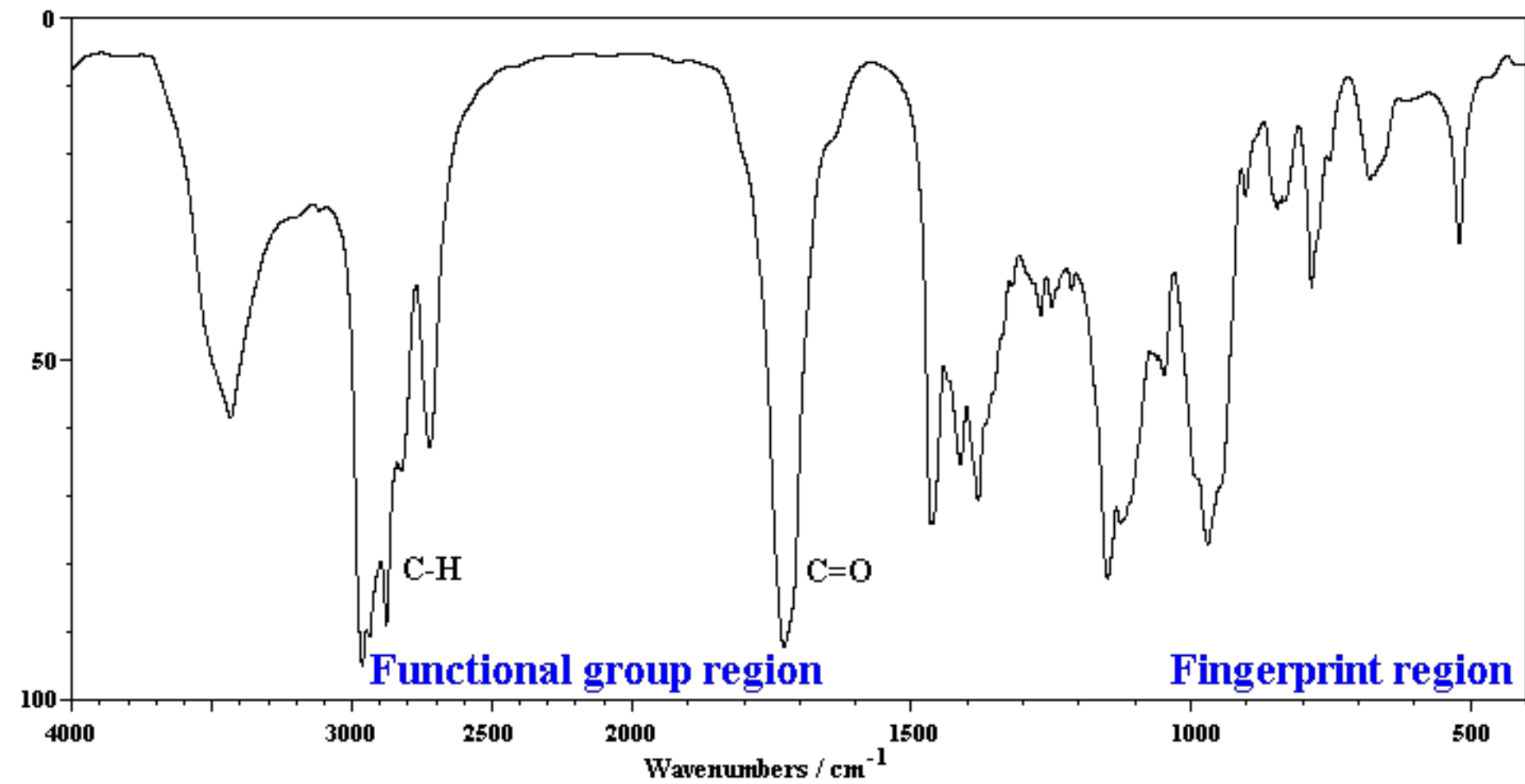
λ (nm)	ϵ (cm ² mol ⁻¹)
240	24 000
280	400
430	20



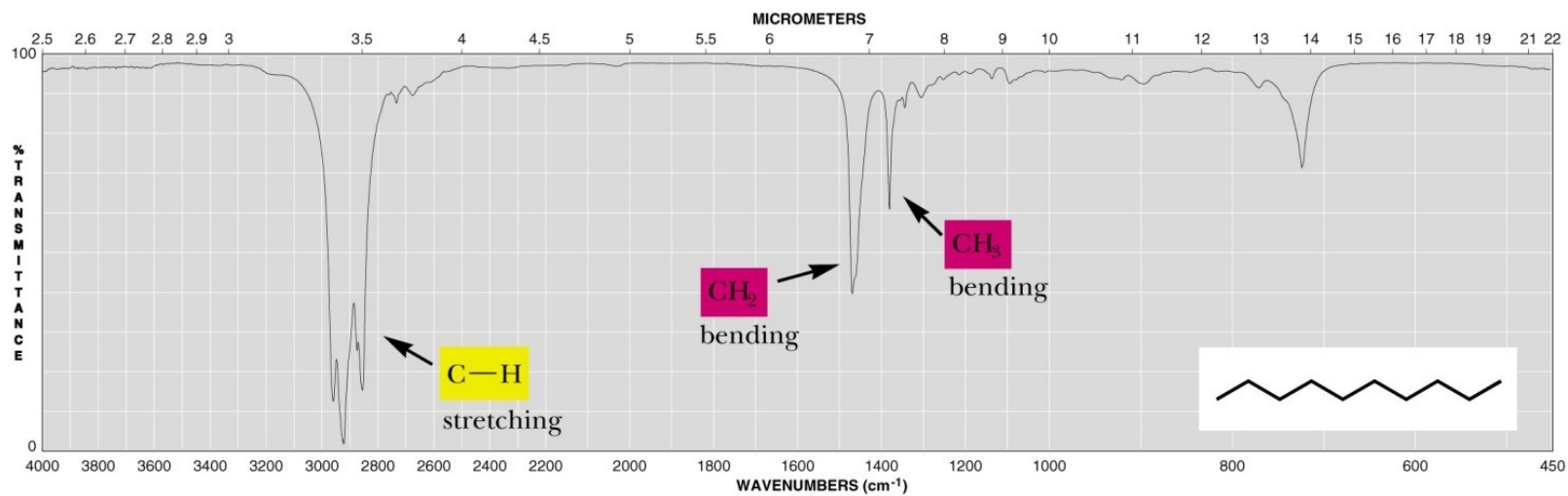
Κίτρινο χρώμα

Ασκήσεις FTIR Spectra

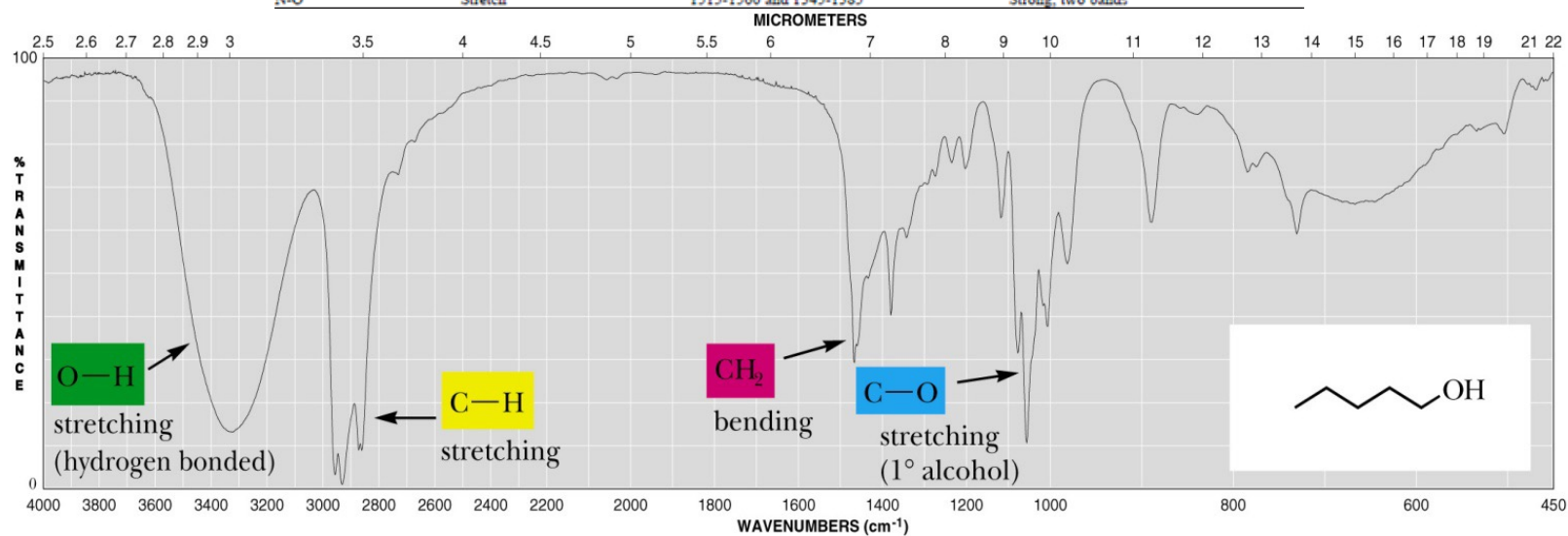
Absorbance / %



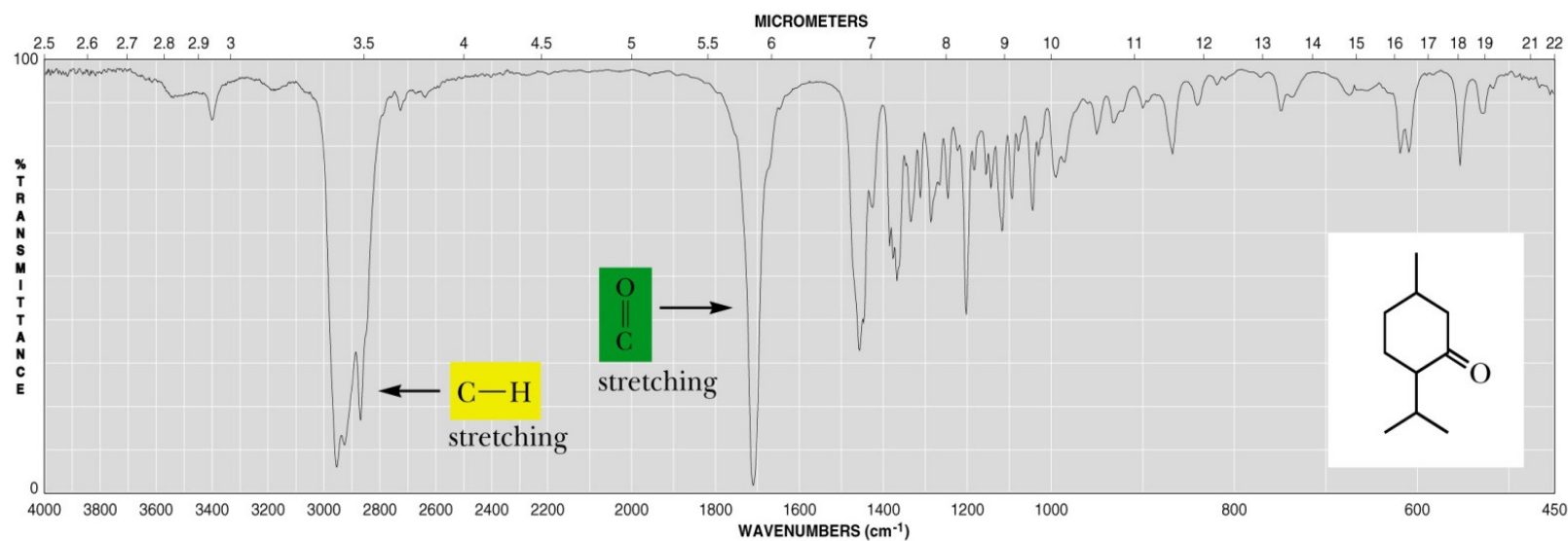
Functional group	Type of vibration	Characteristic absorptions (cm ⁻¹)	Intensity
Alcohol			
O-H	Stretch, H-bonded	3200-3600	Strong, broad
O-H	Stretch, free	3500-3700	Strong, sharp
C-O	Stretch	1050-1150	Strong
Alkane			
C-H	Stretch	2850-3000	Strong
-C-H	Bending	1350-1480	Variable
Alkene			
=C-H	Stretch	3010-3100	Medium
=C-H	Bending	675-1000	Strong
C=C	Stretch	1620-1680	Variable
Alkyl halide			
C-F	Stretch	1000-1400	Strong
C-Cl	Stretch	600-800	Strong
C-Br	Stretch	500-600	Strong
C-I	Stretch	500	Strong
Alkyne			
C-H	Stretch	3300	Strong, sharp
C≡C	Stretch	2100-2260	Variable, not present in symmetrical alkynes
Amine			
N-H	Stretch	3300-3500	Medium (primary amines have two bands; secondary have one band, often very weak)
C-N	Stretch	1080-1360	Medium-weak
N-H	Bending	1600	Medium
Aromatic			
C-H	Stretch	3000-3100	Medium
C=C	Stretch	1400-1600	Medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns:			
Carbonyl			
C=O	Stretch	1670-1820	Strong (conjugation moves absorptions to lower wave numbers)
Ether			
C-O	Stretch	1000-1300 (1070-1150)	Strong
Nitrile			
C-N	Stretch	2210-2260	Medium
Nitro			
N-O	Stretch	1515-1560 and 1345-1385	Strong, two bands



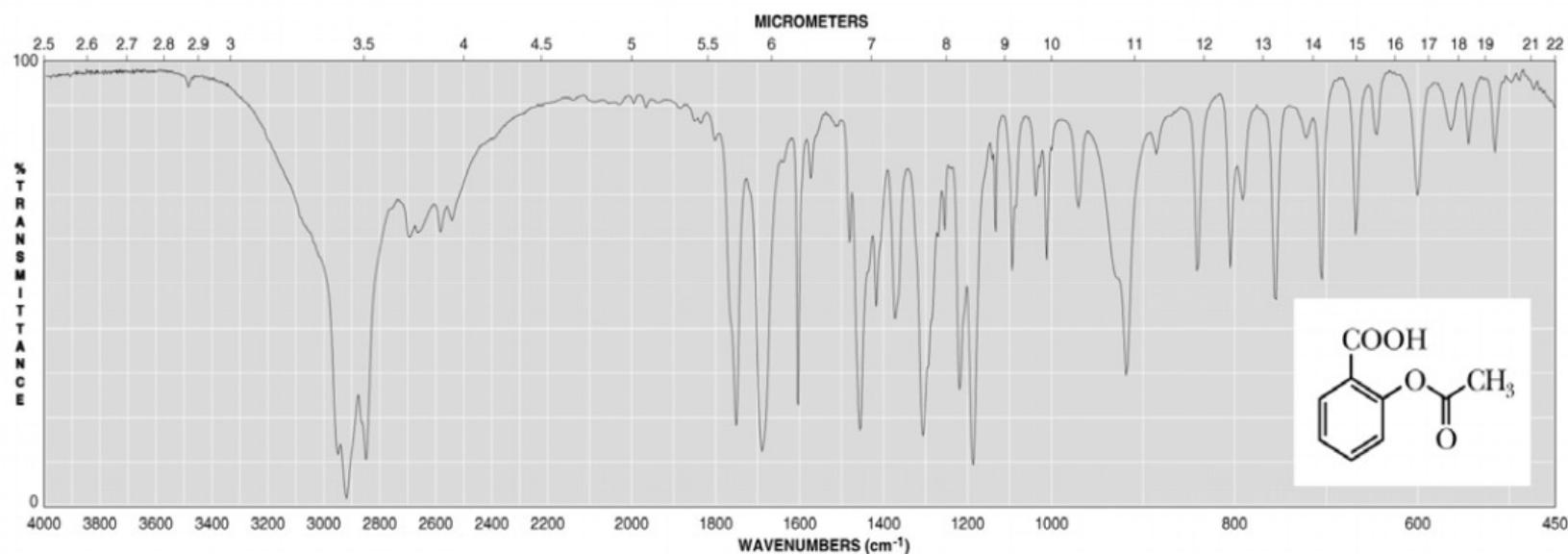
Functional group	Type of vibration	Characteristic absorptions (cm ⁻¹)	Intensity
Alcohol			
O-H	Stretch, H-bonded	3200-3600	Strong, broad
O-H	Stretch, free	3500-3700	Strong, sharp
C-O	Stretch	1050-1150	Strong
Alkane			
C-H	Stretch	2850-3000	Strong
-C-H	Bending	1350-1480	Variable
Alkene			
=C-H	Stretch	3010-3100	Medium
=C-H	Bending	675-1000	Strong
C=C	Stretch	1620-1680	Variable
Alkyl halide			
C-F	Stretch	1000-1400	Strong
C-Cl	Stretch	600-800	Strong
C-Br	Stretch	500-600	Strong
C-I	Stretch	500	Strong
Alkyne			
C-H	Stretch	3300	Strong, sharp
C≡C	Stretch	2100-2260	Variable, not present in symmetrical alkynes
Amine			
N-H	Stretch	3300-3500	Medium (primary amines have two bands; secondary have one band, often very weak)
C-N	Stretch	1080-1360	Medium-weak
N-H	Bending	1600	Medium
Aromatic			
C-H	Stretch	3000-3100	Medium
C=C	Stretch	1400-1600	Medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns:			
Carbonyl			
C=O	Stretch	1670-1820	Strong (conjugation moves absorptions to lower wave numbers)
Ether			
C-O	Stretch	1000-1300 (1070-1150)	Strong
Nitrile			
C-N	Stretch	2210-2260	Medium
Nitro			
N-O	Stretch	1515-1560 and 1345-1385	Strong, two bands



Functional group	Type of vibration	Characteristic absorptions (cm ⁻¹)	Intensity
Alcohol			
O-H	Stretch, H-bonded	3200-3600	Strong, broad
O-H	Stretch, free	3500-3700	Strong, sharp
C-O	Stretch	1050-1150	Strong
Alkane			
C-H	Stretch	2850-3000	Strong
C-H	Bending	1350-1480	Variable
Alkene			
=C-H	Stretch	3010-3100	Medium
=C-H	Bending	675-1000	Strong
C=C	Stretch	1620-1680	Variable
Alkyl halide			
C-F	Stretch	1000-1400	Strong
C-Cl	Stretch	600-800	Strong
C-Br	Stretch	500-600	Strong
C-I	Stretch	500	Strong
Alkyne			
C-H	Stretch	3300	Strong, sharp
C≡C	Stretch	2100-2260	Variable, not present in symmetrical alkynes
Amine			
N-H	Stretch	3300-3500	Medium (primary amines have two bands; secondary have one band, often very weak)
C-N	Stretch	1080-1360	Medium-weak
N-H	Bending	1600	Medium
Aromatic			
C-H	Stretch	3000-3100	Medium
C=C	Stretch	1400-1600	Medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns:			
Carbonyl			
C=O	Stretch	1670-1820	Strong (conjugation moves absorptions to lower wave numbers)
Ether			
C-O	Stretch	1000-1300 (1070-1150)	Strong
Nitrile			
C≡N	Stretch	2210-2260	Medium
Nitro			
N-O	Stretch	1515-1560 and 1345-1385	Strong, two bands



Functional group	Type of vibration	Characteristic absorptions (cm ⁻¹)	Intensity
Alcohol			
O-H	Stretch, H-bonded	3200-3600	Strong, broad
O-H	Stretch, free	3500-3700	Strong, sharp
C-O	Stretch	1050-1150	Strong
Alkane			
C-H	Stretch	2850-3000	Strong
-C-H	Bending	1350-1480	Variable
Alkene			
=C-H	Stretch	3010-3100	Medium
=C-H	Bending	675-1000	Strong
C=C	Stretch	1620-1680	Variable
Alkyl halide			
C-F	Stretch	1000-1400	Strong
C-Cl	Stretch	600-800	Strong
C-Br	Stretch	500-600	Strong
C-I	Stretch	500	Strong
Alkyne			
C-H	Stretch	3300	Strong, sharp
C≡C	Stretch	2100-2260	Variable, not present in symmetrical alkynes
Amine			
N-H	Stretch	3300-3500	Medium (primary amines have two bands; secondary have one band, often very weak)
			Medium-weak
			Medium
C-N	Stretch	1080-1360	
N-H	Bending	1600	
Aromatic			
C-H	Stretch	3000-3100	Medium
C=C	Stretch	1400-1600	Medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns:			
Carbonyl			
C=O	Stretch	1670-1820	Strong (conjugation moves absorptions to lower wave numbers)
Ether			
C-O	Stretch	1000-1300 (1070-1150)	Strong
Nitrile			
C-N	Stretch	2210-2260	Medium
Nitro			
N-O	Stretch	1515-1560 and 1345-1385	Strong, two bands



Aspirin

Aspirin

Functional group	Type of vibration	Characteristic absorptions (cm ⁻¹)	Intensity
Alcohol			
O-H	Stretch, H-bonded	3200-3600	Strong, broad
O-H	Stretch, free	3500-3700	Strong, sharp
C-O	Stretch	1050-1150	Strong
Alkane			
C-H	Stretch	2850-3000	Strong
C-H	Bending	1350-1480	Variable
Alkene			
=C-H	Stretch	3010-3100	Medium
=C-H	Bending	675-1000	Strong
C=C	Stretch	1620-1680	Variable
Alkyl halide			
C-F	Stretch	1000-1400	Strong
C-Cl	Stretch	600-800	Strong
C-Br	Stretch	500-600	Strong
C-I	Stretch	500	Strong
Alkyne			
C-H	Stretch	3300	Strong, sharp
C≡C	Stretch	2100-2260	Variable, not present in symmetrical alkynes
Amine			
N-H	Stretch	3300-3500	Medium (primary amines have two bands; secondary have one band, often very weak)
C-N	Stretch	1080-1360	Medium-weak
N-H	Bending	1600	Medium
Aromatic			
C-H	Stretch	3000-3100	Medium
C=C	Stretch	1400-1600	Medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns:			
Carbonyl			
C=O	Stretch	1670-1820	Strong (conjugation moves absorptions to lower wave numbers)
Ether			
C-O	Stretch	1000-1300 (1070-1150)	Strong
Nitrile			
C≡N	Stretch	2210-2260	Medium
Nitro			
N-O	Stretch	1515-1560 and 1345-1385	Strong, two bands

