

Molecular Vibrations and Corresponding Energy



Vibration Frequency and Bond Strength



Reduced masses are similar; X-H $\overline{\nu}$ dominated by bond strength.

Not hydrogen bonded 12-3

Interpreting Infrared Spectra

D0									
80 - 60 - 40 - 20 -	N—Н О—Н С—Н	C≡N C≡C		C=0 C=N Fingerprint region C=C					
4000	3500 3000	2500	2000 Table 12.1	Chara	1500 1000 acteristic IB Absorpti	ons of Some Function	500		
			Functional Gr	oup	Absorption (cm ⁻¹)	Intensity	Functional Group	Absorption (cm ⁻¹)	Intensity
			Alkane				Amine		
			C-H		2850-2960	Medium	N-H	3300-3500	Medium
			Alkene				C-N	1030-1230	Medium
			=C-H		3020-3100	Medium	Carbonyl compo	ind	
			C=C		1640-1680	Medium	C=0	1670-1780	Strong
			Alkyne				Carboxylic acid		
			=C-H		3300	Strong	O-H	2500-3100	Strong, broad
			C=C		2100-2260	Medium	Nitrile		
			Alkyl halide	8			C=N	2210-2260	Medium
			C-CI		600-800	Strong	Nitro		
			C-Br		500-600	Strong	NO ₂	1540	Strong
			Alcohol						
			O-H		3400-3650	Strong, broad			
			C-0		1050-1150	Strong			
			Arene						
			C-H		3030	Weak			
			Aromatic	ring	1660-2000	Weak			
					1450-1600	Medium			



IR Absorptions of an Alkane



Characteristic IR Absorptions



Examples





Hydrogen Bonding Broadens and Shifts the Absorption Band



Alkyne Stretching Vibrations



Molecular Interpretation of IR Data







Mass Spectroscopy: Measuring the Molecular Mass





Mass Spectra

		exact	mass of four compounds with $m/z = 98$							
Isotope	Mass	C	н	СНО	СНО	СНИ				
¹ H	1.00783	0	7 ' ' 14	0 ₆ 11 ₁₀ 0	05 ¹ ₆ 0 ₂	$O_5 I_{10} I_2$				
¹² C	12.00000	98.	1096	98.0732	98.0368	98.0845				
¹⁴ N	14.0031			1.0		(10010)				
¹⁶ O	15.9949	Requires high-resolution mass spectrometry (HRMS)								
³² S	31.9721					63				
³⁵ Cl	34.9689		100 -							
³⁷ Cl	36.9659		-							
⁷⁹ Br	78.9183				СН	3CH2CH2Br				
⁸¹ Br	80.9163		ndanc							
			ve abu			in the states				
The nearly e	qual heights o	f the peaks	Relati			$124(C_3H_7^{01}Br)$				
at <i>m/z</i> = 122	and 124 are o	due to the	_							
almost equa	l abundances		-							
biomine isot	opes ("Br and	i ′°Bſ).	0	20 40	60 8	80 100 120				
					m/z					