

Answers to Problems Introduction to Spectroscopy, 4th edition

Pavia, Lampman, Kriz, Vyvyan

CHAPTER 1

(a)

(b)

1.

1.	(a)	90.509	% carbo	n; 9.50	% hydr	ogen	(b)	C_4H_5		
2.	32.0% carbon; 5.4% hydrogen; 62.8% chlorine; C ₃ H ₆ Cl ₂									
3.	$C_2H_5NO_2$									
4.	$180.2 = \text{molecular mass.}$ Molecular formula is $C_9H_8O_4$.									
5.	Equivalent weight = 52.3									
6.	(a)	6	(b)	1	(c)	3	(d)	6	(e)	12
7.	The index of hydrogen deficiency = 1. There cannot be a triple bond, since the presence of a triple bond would require an index of hydrogen deficiency of at least 2.									
8.	(a) 59.96% carbon; 5.75% hydrogen; 34.29% oxygen (b) C ₇ H ₈ O ₃ (c) C ₂₁ H ₂₄ O ₉ (d) A maximum of two aromatic (benzenoid) rings									
9.	(a) $C_8H_8O_2$ (b) $C_8H_{12}N_2$ (c) $C_7H_8N_2O$ (d) $C_5H_{12}O_4$									
10.	Molecular formula = $C_8H_{10}N_4O_2$; index of hydrogen deficiency = 6									
11.	Molecular formula = $C_{21}H_{30}O_2$; index of hydrogen deficiency = 7									
12.	For the hydrolysis product: molecular formula = $C_6H_{12}O_6$; index of hydrogen deficiency = 1									
	For the original carbohydrate: molecular formula = $C_{12}H_{22}O_{11}$; index of hydrogen deficiency = 2									
CHAPTER 2										

Propargyl chloride (3-chloropropyne)

p-Cymene (4-isopropyltoluene)

- (c) *m*-Toluidine (3-methylaniline)
- (d) *o*-Cresol (2-methylphenol)
- (e) *N*-Ethylaniline
- (f) 2-Chlorotoluene
- (g) 2-Chloropropanoic acid
- (h) 3-Methyl-1-butanol
- (i) 5-Hexen-2-one
- (j) 1,2,3,4-Tetrahydronaphthalene
- (k) 3-(Dimethylamino)propanenitrile
- (1) 1,2-Epoxybutane
- 2. Citronellal
- 3. *trans*-Cinnamaldehyde (*trans*-3-phenyl-2-propenal)
- 4. Upper spectrum, *trans*-3-hexen-1-ol; Lower spectrum, *cis*-3-hexen-1-ol
- 5. (a) Structure B (ethyl cinnamate)
 - (b) Structure C (cyclobutanone)
 - (c) Structure D (2-ethylaniline)
 - (d) Structure A (propiophenone)
 - (e) Structure D (butanoic anhydride)
 - (f) Structure C (Carvone)
 - (g) Structure B (undecylenic aldehyde)
 - (h) Structure D (2-ethyl-*trans*-2-hexenal)
 - (i) Structure B (*N*-methylcyclohexylamine)
 - (j) Structure B (1-hexanethiol)
- 6. Poly(acrylonitrile-styrene); poly(methyl methacrylate); polyamide (nylon)
- 7. Propyl acetate, allyl acetate, and ethyl acrylate
- 8. 2-Ethyl-δ-valerolactone, 3,4-dihydro-6-methyl-2*H*-pyran-2-one, and 5,6-dihydro-2*H*-pyran-2-one
- 9. α -Methylene- γ -butyrolactone, γ -methylene- γ -butyrolactone, and γ -valerolactone
- 10. 4-Penten-1-ol, 3-methyl-2-buten-1-ol, and 3-methyl-3-buten-1-ol
- 11. Resonance effect: the amino group pushes electron density into the ring and into the carbonyl group resulting in a lower frequency carbonyl group (more single bond character). A nitro group withdraws electrons resulting in higher frequency carbonyl absorption (more double bond character).