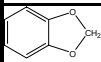


Universidad de Chile
 Facultad de Ciencias Químicas y Farmacéuticas
 Departamento de Química Orgánica y Fisicoquímica

COMPUESTOS HETEROCICLICOS Y ANALISIS ESTRUCTURAL

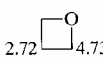
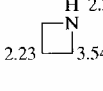
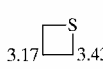
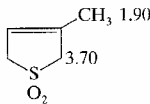
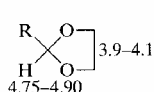
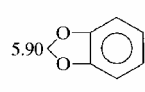
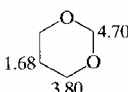
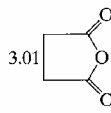
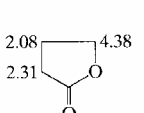
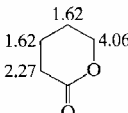
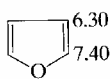
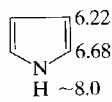
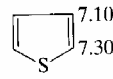
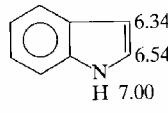
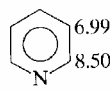
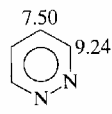
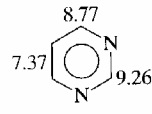
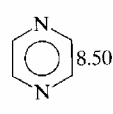
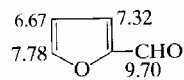
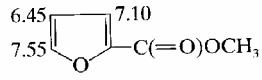
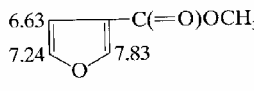
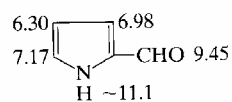
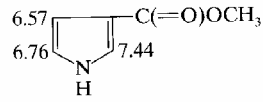
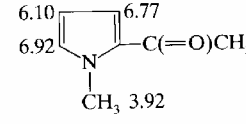
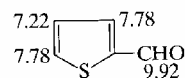
Tabla ^1H -RMN
 Profesora Carolina Jullian

METILO	METILENO	METINO	OTROS
Grupo δ ,ppm	Grupo δ ,ppm	Grupo δ ,ppm	Grupo δ ,ppm
$\text{CH}_3\text{-C}$ 0.9	$\text{C-CH}_2\text{-C}$ 1.4	C-CH-C 1.5	H-N 1 –3
$\text{CH}_3\text{-C-C-C=C}$ 1.1	$\text{C-CH}_2\text{-C-C=C}$ 1.7	C-CH-C-O 2.0	H-OR 1 –5
$\text{CH}_3\text{-C-O}$ 1.3	$\text{C-CH}_2\text{-C-O}$ 1.9	C-CH-C=C- 2.4	$\text{H-C}\equiv\text{C-}$ 2.5
$\text{CH}_3\text{-C=C}$ 1.6	$\text{C-CH}_2\text{-C=C}$ 2.3	C-CH-Ar 3.0	H-C=C 5.5
$\text{CH}_3\text{C=O}$ 2.1	$\text{C-CH}_2\text{-Ar}$ 2.7	C-CH-CO-R 2.7	H-Ar 7.3
$\text{CH}_3\text{-Ar}$ 2.3	$\text{C-CH}_2\text{-CO-R}$ 2.4	C-CH-CO-Ar 3.3	H-C=O 10.0
$\text{CH}_3\text{-CO-Ar}$ 2.6	$\text{C-CH}_2\text{-CO-O-R}$ 2.2	C-CH-OR 3.7	H-O-C=O 9 -12
$\text{CH}_3\text{-CO-O-R}$ 2.0	$\text{C-CH}_2\text{-CO-N-R}$ 2.2	C-CH-OH 3.9	
$\text{CH}_3\text{-CO-O-Ar}$ 2.4	$\text{C-CH}_2\text{-O-R}$ 3.4	C-CH-O-CO-R 4.8	
$\text{CH}_3\text{-CO-N-R}$ 2.0	$\text{C-CH}_2\text{-O-H}$ 3.6	C-CH-NR_2 2.9	
$\text{CH}_3\text{-O-R}$ 3.3	$\text{C-CH}_2\text{-O-Ar}$ 4.3	C-CH-S 3.2	
$\text{CH}_3\text{-O-C=C}$ 3.8	$\text{C-CH}_2\text{-O-CO-R}$ 4.1	C-CH-NO_2 4.7	
$\text{CH}_3\text{-O-Ar}$ 3.8	$\text{C-CH}_2\text{-N}$ 2.5	C-CH-Br 4.3	
$\text{CH}_3\text{-O-CO-R}$ 3.7	$\text{C-CH}_2\text{-S}$ 2.4	C-CH-I 4.3	
$\text{CH}_3\text{-NR}_2$ 2.2	$\text{C-CH}_2\text{-NO}_2$ 4.4	$\text{C-CH-C}\equiv\text{N}$ 2.7	
$\text{CH}_3\text{-N}$ 2.3	$\text{C-CH}_2\text{-C-NO}_2$ 4.4	C-CH-N-CO-R 4.1	
$\text{CH}_3\text{-N-Ar}$ 3.0	$\text{C-CH}_2\text{-C=C-CO}$ 2.4		
$\text{CH}_3\text{-S}$ 2.1	$\text{C=C(CH}_2\text{)-CO}$ 2.4		
$\text{CH}_3\text{-C-NO}_2$ 1.6	$\text{C-CH}_2\text{-Cl}$ 3.6		
$\text{CH}_3\text{-C=C-CO}$ 2.0	$\text{C-CH}_2\text{-Br}$ 3.5		
$\text{C=C(CH}_3\text{)CO}$ 1.8	$\text{C-CH}_2\text{-I}$ 3.2		
$\text{CH}_3\text{-N-CO-R}$ 2.9	$\text{C-CH}_2\text{-C}\equiv\text{N}$ 2.3		
$\text{CH}_3\text{-Br}$ 2.7	 5.9		
$\text{CH}_3\text{-Cl}$ 3.1			
$\text{CH}_3\text{-N+}$ 3.3			

Appendix F Proton Spin-Coupling Constants

Type	J_{ab} (Hz)	J_{ab} Typical	Type	J_{ab} (Hz)	J_{ab} Typical
	0-30	12-15		4-10	7
CH _a -CH _b (free rotation)	6-8	7		0-3	1.5
	0-1	0		0-3	2
			C=CH _a -CH _b =C 	9-13 3 member 4 member 5 member 6 member 7 member 8 member	10 0.5-2.0 2.5-4.0 5.1-7.0 8.8-11.0 9-13 10-13
ax-ax	6-14	8-10			
ax-eq	0-5	2-3			
eq-eq	0-5	2-3			
	cis 5-10 trans 5-10		CH _a -C≡CH _b -CH _a -C≡C-CH _b -	2-3 2-3	
(cis or trans)					6
	cis 4-12 trans 2-10				4
(cis or trans)					2.5
	cis 7-13 trans 4-9			J (ortho) 6-10 J (meta) 1-3 J (para) 0-1	9 3 ~0
(cis or trans)					
CH _a -OH _b (no exchange)	4-10	5		J (2-3) 5-6 J (3-4) 7-9 J (2-4) 1-2 J (3-5) 1-2 J (2-5) 0-1 J (2-6) 0-1	5 8 1.5 1.5 1 ~0
	1-3	2-3		J (2-3) 1.3-2.0 J (3-4) 3.1-3.8 J (2-4) 0-1 J (2-5) 1-2	5 8 ~0 1.5
	5-8	6		J (2-3) 4.9-6.2 J (3-4) 3.4-5.0 J (2-4) 1.2-1.7 J (2-5) 3.2-3.7	5 8 ~0 1.5
	12-18	17			5.4 4.0 1.5 3.4
	0-3	0-2			
	6-12	10			
	0-3	1-2			
	J (1-2) J (1-3) J (2-3) J (3-4) J (2-4) J (2-5)	2-3 2-3 2-3 3-4 1-2 1.5-2.5			
	J (4-5) J (2-5) J (2-4) J (4-6)	4-6 1-2 0-1 2-3			
	J (4-5) J (2-5) J (2-4)	3-4 1-2 ~0			

Table C.2 Chemical Shifts in Heterocyclic Rings

 2.54	 2.72 4.73	 1.85 3.75	 1.51 3.52	
 1.62 H 0.03	 H 2.38 2.23 3.54	 1.59 N 2.75 H 2.01	 1.50 N 2.74 H 1.84	
 2.27	 3.17 3.43	 1.93 2.82	 2.23 3.00	 CH ₃ 1.90 3.70
 R 3.9-4.1 H 4.75-4.90	 5.90	 1.68 3.80	 3.55	
 3.01	 2.08 4.38 2.31	 1.62 4.06 2.27		
 6.30 7.40	 6.22 6.68 H ~8.0	 7.10 7.30	 6.34 6.54 H 7.00	
 6.99 8.50	 7.50 9.24	 7.37 8.77 9.26	 8.50	
 6.67 7.32 7.78 9.70	 6.45 7.10 7.55	 6.63 7.24 7.83		
 6.30 6.98 7.17 9.45 H ~11.1	 6.57 7.44 H	 6.10 6.77 6.92 3.92 CH ₃		
	 7.22 7.78 7.78 9.92 CHO			