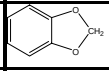
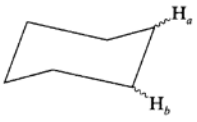
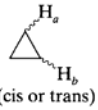
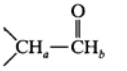
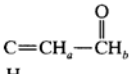
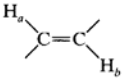
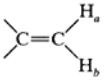
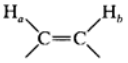
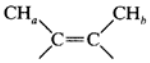
Universidad de Chile
Facultad de Ciencias Químicas y Farmacéuticas
Departamento de Química Orgánica y Fisicoquímica

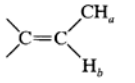
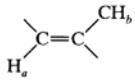
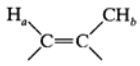
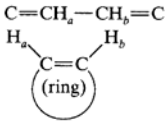
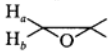
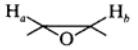
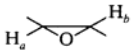
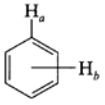
COMPUESTOS HETEROCICLICOS Y ANALISIS ESTRUCTURAL

Tabla ^{1}H-RMN
Profesora Carolina Jullian

METILO		METILENO		METINO		OTROS	
Grupo	δ,ppm	Grupo	δ,ppm	Grupo	δ,ppm	Grupo	δ,ppm
CH_3-C	0.9	C-CH_2-C	1.4	C-CH-C	1.5	H-N	1 –3
CH_3-C-C-C=C	1.1	C-CH_2-C-C=C	1.7	C-CH-C-O	2.0	H-OR	1 –5
CH_3-C-O	1.3	C-CH_2-C-O	1.9	C-CH-C=C-	2.4	H-C≡C-	2.5
CH_3-C=C	1.6	C-CH_2-C=C	2.3	C-CH-Ar	3.0	H-C=C	5.5
CH_3C=O	2.1	C-CH_2-Ar	2.7	C-CH-CO-R	2.7	H-Ar	7.3
CH_3-Ar	2.3	C-CH_2-CO-R	2.4	C-CH-CO-Ar	3.3	H-C=O	10.0
CH_3-CO-Ar	2.6	C-CH_2-CO-O-R	2.2	C-CH-OR	3.7	H-O-C=O	9 -12
CH_3-CO-O-R	2.0	C-CH_2-CO-N-R	2.2	C-CH-OH	3.9		
CH_3-CO-O-Ar	2.4	C-CH_2-O-R	3.4	C-CH-O-CO-R	4.8		
CH_3-CO-N-R	2.0	C-CH_2-O-H	3.6	C-CH-NR_2	2.9		
CH_3-O-R	3.3	C-CH_2-O-Ar	4.3	C-CH-S	3.2		
CH_3-O-C=C	3.8	C-CH_2-O-CO-R	4.1	C-CH-NO_2	4.7		
CH_3-O-Ar	3.8	C-CH_2-N	2.5	C-CH-Br	4.3		
CH_3-O-CO-R	3.7	C-CH_2-S	2.4	C-CH-I	4.3		
CH_3-NR_2	2.2	C-CH_2-NO_2	4.4	C-CH-C≡N	2.7		
CH_3-N	2.3	C-CH_2-C-NO_2	4.4	C-CH-N-CO-R	4.1		
CH_3-N-Ar	3.0	C-CH_2-C=C-CO	2.4				
CH_3-S	2.1	C=C(CH_2)-CO	2.4				
CH_3-C-NO_2	1.6	C-CH_2-Cl	3.6				
CH_3-C=C-CO	2.0	C-CH_2-Br	3.5				
C=C(CH_3)CO	1.8	C-CH_2-I	3.2				
CH_3-N-CO-R	2.9	C-CH_2-C≡N	2.3				
CH_3-Br	2.7		5.9				
CH_3-Cl	3.1						
CH_3-N+-	3.3						

Appendix F Proton Spin-Coupling Constants

Type	J_{ab} (Hz)	J_{ab} Typical
	0–30	12–15
CH_a-CH_b (free rotation)	6–8	7
	0–1	0
		
ax–ax	6–14	8–10
ax–eq	0–5	2–3
eq–eq	0–5	2–3
 (cis or trans)	*cis* 5–10 *trans* 5–10	
 (cis or trans)	*cis* 4–12 *trans* 2–10	
 (cis or trans)	*cis* 7–13 *trans* 4–9	
CH_a-OH_b (no exchange)	4–10	5
	1–3	2–3
	5–8	6
	12–18	17
	0–3	0–2
	6–12	10
	0–3	1–2

Type	J_{ab} (Hz)	J_{ab} Typical
	4–10	7
	0–3	1.5
	0–3	2
	9–13	10
	3 member	0.5–2.0
	4 member	2.5–4.0
	5 member	5.1–7.0
	6 member	8.8–11.0
	7 member	9–13
	8 member	10–13
$CH_a-C\equiv CH_b$	2–3	
$-CH_a-C\equiv C-CH_b-$	2–3	
		6
		4
		2.5
	*J* (ortho) 6–10 *J* (meta) 1–3 *J* (para) 0–1	9 3 ~0
	*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
	*J* (2–3) 1.3–2.0 *J* (3–4) 3.1–3.8 *J* (2–4) 0–1 *J* (2–5) 1–2	1.8 3.6 ~0 1.5
	*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	5.4 4.0 1.5 3.4

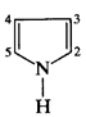
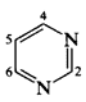
	*J* (1–2)	2–3
	J (1–3)	2–3
	J (2–3)	2–3
	J (3–4)	3–4
	J (2–4)	1–2
	J (2–5)	1.5–2.5
	*J* (4–5)	4–6
	J (2–5)	1–2
	J (2–4)	0–1
	J (4–6)	2–3
	*J* (4–5)	3–4
	J (2–5)	1–2
	J (2–4)	~0

Table C.2 Chemical Shifts in Heterocyclic Rings