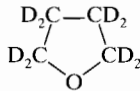
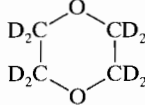
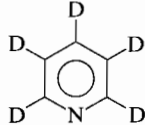


THE ¹³C CHEMICAL SHIFTS, COUPLINGS, AND MULTIPLICITIES APPENDIX A OF COMMON NMR SOLVENTS

Structure	Name	δ (ppm)	J_{C-D} (Hz)	Multiplicity ^a
CDCl ₃	Chloroform- <i>d</i> ₁	77.0	32	Triplet
CD ₃ OD	Methanol- <i>d</i> ₄	49.0	21.5	Septet
CD ₃ SOCD ₃	DMSO- <i>d</i> ₆	39.7	21	Septet
	DMF- <i>d</i> ₇	30.1	21	Septet
		35.2	21	Septet
		167.7	30	Triplet
C ₆ D ₆	Benzene- <i>d</i> ₆	128.0	24	Triplet
	THF- <i>d</i> ₈	25.2	20.5	Quintet
		67.4	22	Quintet
	Dioxane- <i>d</i> ₈	66.5	22	Quintet
	Pyridine- <i>d</i> ₅	123.5 (C-3,5)	25	Triplet
		135.5 (C-4)	24.5	Triplet
		149.2 (C-2,6)	27.5	Triplet
	Acetone- <i>d</i> ₆	29.8 (methyl)	20	Septet
		206.5 (carbonyl)	<1	Septet ^b
CD ₃ CN	Acetonitrile- <i>d</i> ₃	1.3 (methyl)	32	Septet
		118.2 (CN)	<1	Septet ^b
CD ₃ NO ₂	Nitromethane- <i>d</i> ₃	60.5	23.5	Septet
CD ₃ CD ₂ OD	Ethanol- <i>d</i> ₆	15.8 (C-2)	19.5	Septet
		55.4 (C-1)	22	Quintet
(CD ₃ CD ₂) ₂ O	Ether- <i>d</i> ₁₀	13.4 (C-2)	19	Septet
		64.3 (C-1)	21	Quintet
[(CD ₃) ₂ N] ₃ P=O	HMPA- <i>d</i> ₁₈	35.8	21	Septet
CD ₃ CO ₂ D	Acetic acid- <i>d</i> ₄	20.2 (C-2)	20	Septet
		178.4 (C-1)	<1	Septet ^b
CD ₂ Cl ₂	Dichloromethane- <i>d</i> ₂ (Methylene chloride- <i>d</i> ₂)	53.1	29	Quintet

^a Triplet intensities = 1:1:1, quintet = 1:2:3:2:1, septet = 1:3:6:7:6:3:1.

^b Unresolved, long-range coupling.

Source: Breitmaier, E., and Voelter, W. (1987). *Carbon-13 NMR Spectroscopy*, 3rd ed. New York: VCH, p. 109; with permission. Also Merck & Co., Inc.

Table 2. $^{13}\text{C}\{^1\text{H}\}$ NMR Data^a

	carbon	THF- <i>d</i> ₈	CD ₂ Cl ₂	CDCl ₃	toluene- <i>d</i> ₈	C ₆ D ₆	C ₆ D ₅ Cl	(CD ₃) ₂ CO	(CD ₃) ₂ SO	CD ₃ CN	TFE- <i>d</i> ₃	CD ₃ OD	D ₂ O
solvent signals		67.21 25.31	53.84	77.16	137.48 128.87 127.96 125.13 20.43	128.06	134.19 129.26 128.25 125.96	29.84 206.26	39.52	1.32 118.26	61.50 126.28	49.00	
acetic acid	CO	171.69	175.85	175.99	175.30	175.82	175.67	172.31	171.93	173.21	177.96	175.11	177.21
	CH ₃	20.13	20.91	20.81	20.27	20.37	20.40	20.51	20.95	20.73	20.91	20.56	21.03
acetone	CO	204.19	206.78	207.07	204.00	204.43	204.83	205.87	206.31	207.43	32.35	209.67	215.94
	CH ₃	30.17	31.00	30.92	30.03	30.14	30.12	30.60	30.56	30.91	214.98	30.67	30.89
acetonitrile	CN	116.79	116.92	116.43	115.76	116.02	115.93	117.60	117.91	118.26	118.95	118.06	119.68
	CH ₃	0.45	2.03	1.89	0.03	0.20	0.63	1.12	1.03	1.79	1.00	0.85	1.47
benzene	CH	128.84	128.68	128.37	128.57	128.62	128.38	129.15	128.30	129.32	129.84	129.34	
<i>tert</i> -butyl alcohol	(CH ₃) ₃ C	67.50	69.11	69.15	68.12	68.19	68.19	68.13	66.88	68.74	72.35	69.40	70.36
	(CH ₃) ₃ C	30.57	31.46	31.25	30.49	30.47	31.13	30.72	30.38	30.68	31.07	30.91	30.29
carbon dioxide	CO ₂	125.69	125.26	124.99	124.86	124.76	126.08	125.81	124.21	125.89	126.92	126.31	
carbon disulfide	CS ₂	193.37	192.95	192.83	192.71	192.69	192.49	193.58	192.63	193.60	196.26	193.82	197.25
carbon tetrachloride	CCl ₄	96.89	96.52	96.34	96.57	96.44	96.38	96.65	95.44	96.68	97.74	97.21	96.73
chloroform	CH	79.24	77.99	77.36	77.89	77.79	77.67	79.19	79.16	79.17	78.83	79.44	
18-crown-6	CH ₂	71.34	70.47	70.55	70.86	70.59	70.55	71.25	69.85	71.22	70.80	71.47	70.14
cyclohexane	CH ₂	27.58	27.38	26.94	27.31	27.23	26.99	27.51	26.33	27.63	28.34	27.96	
1,2-dichloroethane	CH ₂	44.64	44.35	43.50	43.40	43.59	43.60	45.25	45.02	45.54	45.28	45.11	
dichloromethane	CH ₂	54.67	54.24	53.52	53.47	53.46	53.54	54.95	54.84	55.32	54.46	54.78	
diethyl ether	CH ₃	15.49	15.44	15.20	15.47	15.46	15.35	15.78	15.12	15.63	15.33	15.46	14.77
	CH ₂	66.14	66.11	65.91	65.94	65.94	65.79	66.12	62.05	66.32	67.55	66.88	66.42
diglyme	CH ₃	58.72	58.95	59.01	58.62	58.66	58.42	58.77	57.98	58.90	59.40	59.06	58.67
	CH ₂	71.17	70.70	70.51	70.92	70.87	70.56	71.03	69.54	70.99	73.05	71.33	70.05
	CH ₂	72.72	72.25	71.90	72.39	72.35	72.07	72.63	71.25	72.63	71.33	72.92	71.63
dimethylformamide	CH	161.96	162.57	162.62	161.93	162.13	162.01	162.79	162.29	163.31	166.01	164.73	165.53
	CH ₃	35.65	36.56	36.50	35.22	35.25	35.45	36.15	35.73	36.57	37.76	36.89	37.54
	CH ₃	30.70	31.39	31.45	30.64	30.72	30.71	31.03	30.73	31.32	30.96	31.61	32.03
1,4-dioxane	CH ₂	67.65	67.47	67.14	67.17	67.16	66.95	67.60	66.36	67.72	68.52	68.11	67.19
DME	CH ₃	58.72	59.02	59.08	58.63	58.68	58.31	58.45	58.03	58.89	59.52	59.06	58.67
	CH ₂	72.58	72.24	71.84	72.25	72.21	71.81	72.47	71.17	72.47	72.87	72.72	71.49
ethane	CH ₃	6.79	6.91	6.89	6.94	6.96	6.91	6.88	6.61	6.99	7.01	6.98	
ethanol	CH ₃	18.90	18.69	18.41	18.78	18.72	18.55	18.89	18.51	18.80	18.11	18.40	17.47
	CH ₂	57.60	58.57	58.28	57.81	57.86	57.63	57.72	56.07	57.96	59.68	58.26	58.05
ethyl acetate	CH ₃ CO	20.45	21.15	21.04	20.46	20.56	20.50	20.83	20.68	21.16	21.18	20.88	21.15
	CO	170.32	171.24	171.36	170.02	170.44	170.20	170.96	170.31	171.68	175.55	172.89	175.26
	CH ₂	60.30	60.63	60.49	60.08	60.21	60.06	60.56	59.74	60.98	62.70	61.50	62.32
	CH ₃	14.37	14.37	14.19	14.23	14.19	14.07	14.50	14.40	14.54	14.36	14.49	13.92
ethylene	CH ₂	123.09	123.20	123.13	122.92	122.96	122.95	123.47	123.52	123.69	124.08	123.46	
ethylene glycol	CH ₂	64.35	64.08	63.79	64.29	64.34	64.03	64.26	62.76	64.22	64.87	64.30	63.17
H grease ^b	CH ₂	30.45	30.14	29.71	30.31	30.22	30.11						
hexamethylbenzene	C	131.88	132.09	132.21	131.72	131.79	131.54	132.22	131.10	132.61	134.04	132.53	
	CH ₃	16.71	16.93	16.98	16.84	16.95	16.68	16.86	16.60	16.94	17.04	16.90	
<i>n</i> -hexane	CH ₃	14.22	14.28	14.14	14.34	14.32	14.18	14.34	13.88	14.43	14.63	14.45	
	CH ₂ (2,5)	23.33	23.07	22.70	23.12	23.04	22.86	23.28	22.05	23.40	24.06	23.68	
	CH ₂ (3,4)	32.34	32.01	31.64	32.06	31.96	31.77	32.30	30.95	32.36	33.17	32.73	
HMSO	CH ₃	1.83	1.96	1.97	1.99	2.05	1.92	2.01	1.96	2.07	2.09	1.99	2.31
HMPA ^c	CH ₃	36.89	36.99	36.87	36.80	36.88	36.64	37.04	36.42	37.10	37.21	37.00	36.46
imidazole	CH(2)	135.72	135.76	135.38	135.57	135.76	135.50	135.89	135.15	136.33	136.58	136.31	136.65
	CH(4,5)	122.20	122.16	122.00	122.13	122.16	121.96	122.31	121.55	122.78	122.93	122.60	122.43
methane	CH ₄	-4.90	-4.33	-4.63	-4.34	-4.29	-4.33	-5.33	-4.01	-4.61	-5.88	-4.90	
methanol	CH ₃	49.64	50.45	50.41	49.90	49.97	49.66	49.77	48.59	49.90	50.67	49.86	49.50 ^d
nitromethane	CH ₃	62.49	63.03	62.50	61.14	61.16	61.68	63.21	63.28	63.66	63.17	63.08	63.22
<i>n</i> -pentane	CH ₃	14.18	14.24	14.08	14.27	14.25	14.10	14.29	13.28	14.37	14.54	14.39	
	CH ₂ (2,4)	23.00	22.77	22.38	22.79	22.72	22.54	22.98	21.70	23.08	23.75	23.38	
	CH ₂ (3)	34.87	34.57	34.16	34.54	34.45	34.26	34.83	33.48	34.89	35.76	35.30	
propane	CH ₃	16.60	16.63	16.63	16.65	16.66	16.56	16.68	16.34	16.73	16.93	16.80	
	CH ₂	16.82	16.63	16.37	16.63	16.60	16.48	16.78	15.67	16.91	17.46	17.19	
2-propanol	CH ₃	25.70	25.43	25.14	25.24	25.18	25.14	25.67	25.43	25.55	25.21	25.27	24.38
	CH	66.14	64.67	64.50	64.12	64.23	64.18	63.85	64.92	64.30	66.69	64.71	64.88
propylene	CH ₃	19.27	19.47	19.50	19.32	19.38	19.32	19.42	19.20	19.48	19.63	19.50	
	CH ₂	115.74	115.70	115.74	115.89	115.92	115.86	116.03	116.07	116.12	116.38	116.04	
	CH	134.02	134.21	133.91	133.61	133.69	133.57	134.34	133.55	134.78	136.00	134.61	
pyridine	CH(2,6)	150.57	150.27	149.90	150.25	150.27	149.93	150.67	149.58	150.76	149.76	150.07	149.18
	CH(3,5)	124.08	124.06	123.75	123.46	123.58	123.49	124.57	123.84	127.76	126.27	125.53	125.12
	CH(4)	135.99	136.16	135.96	135.17	135.28	135.32	136.56	136.05	136.89	139.62	138.35	138.27
pyrrole	CH(2,5)	118.03	117.93	117.77	117.61	117.78	117.65	117.98	117.32	118.47	119.61	118.28	119.06
	CH(3,4)	107.74	108.02	107.98	108.15	108.21	108.03	108.04	107.07	108.31	108.85	108.11	107.83
pyrrolidine ^e	CH ₂ (2,5)	45.82	47.02	46.93	47.12	46.86	46.75		46.51	47.57	47.43	47.23	46.83
	CH ₂ (3,4)	26.17	25.83	25.56	25.75	25.65	25.59		25.26	26.34	25.73	26.29	25.86
silicone grease	CH ₃	1.20	1.22	1.19	1.37	1.38	1.09	1.40			2.87	2.10	
tetrahydrofuran	CH ₂ (2,5)	68.03	68.16	67.97	67.75	67.80	67.64	68.07	67.03	68.33	69.53	68.83	68.68
	CH ₂ (3,4)	26.19	25.98	25.62	25.79	25.72	25.68	26.15	25.14	26.27	26.69	26.48	25.67
toluene	CH ₃	21.29	21.53	21.46	21.37	21.10	21.23	21.46	20.99	21.50	21.62	21.50	
	C(1)	138.24	138.36	137.89	137.84	137.91	137.65	138.48	137.35	138.90	139.92	138.85	
	CH(2,6)	129.47	129.35	129.07	129.33	129.33	129.12	129.76	128.88	129.94	130.58	129.91	
	CH(3,5)	128.71	128.54	128.26	128.51	128.56	128.31	129.03	128.18	129.23	129.79	129.20	
	CH(4)	125.84	125.62	125.33	125.66	125.68	125.43	126.12	125.29	126.28	126.82	126.29	
triethylamine	CH ₃	12.51	12.12	11.61	12.39	12.35	11.87	12.49	11.74	12.38	9.51	11.09	9.07
	CH ₂	47.18	46.75	46.25	46.82	46.77	46.36	47.07	45.74	47.10	48.45	46.96	47.19

^a Except for the compounds in solutions 8–10, as well as the gas samples, hexamethylbenzene, and the corrected values mentioned in the Supporting Information, all data for the solvents CDCl₃, C₆D₆, (CD₃)₂CO, (CD₃)₂SO, CD₃CN, CD₃OD, and D₂O were previously reported in ref 2. ^b Apiezon brand H grease. ^c Phosphorus coupling was observed (²J_{PC} = 3 Hz). ^d Internal reference; see text. ^e Pyrrolidine was observed to react with (CD₃)₂CO.

APPENDIX B (Continued)

<i>n</i> -hexane	CH ₃	14.14	14.34	13.88	14.32	14.43	14.45	
	CH ₂ (2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH ₂ (3)	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA	CH ₃	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH ₃	50.41	49.77	48.59	49.97	49.90	49.86	49.50
nitromethane	CH ₃	62.50	63.21	63.28	61.16	63.66	63.08	63.22
<i>n</i> -pentane	CH ₃	14.08	14.29	13.28	14.25	14.37	14.39	
	CH ₂ (2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH ₂ (3)	34.16	34.83	33.48	34.45	34.89	35.30	
2-propanol	CH ₃	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH ₃	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH ₂	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH ₂ O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH ₃	21.46	21.46	20.99	21.10	21.50	21.50	
	C(<i>i</i>)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(<i>o</i>)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(<i>m</i>)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(<i>p</i>)	125.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH ₃	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH ₂	46.25	47.07	45.74	46.77	47.10	46.96	47.19

APPENDIX C THE ¹³C CORRELATION CHART FOR CHEMICAL CLASSES

R = H or alkyl substituents

Y = polar substituents

Acyclic hydrocarbons

-CH₃-CH₂

-CH

-C-

Alicyclic hydrocarbons

C₃H₆C₄H₈ to C₁₀H₂₀

Alkenes

H₂C = C - RH₂C = C - Y

C = C - C = C - R

Allenes

C = C = C

Alkynes

C ≡ C - R

C ≡ C - Y

Aromatics

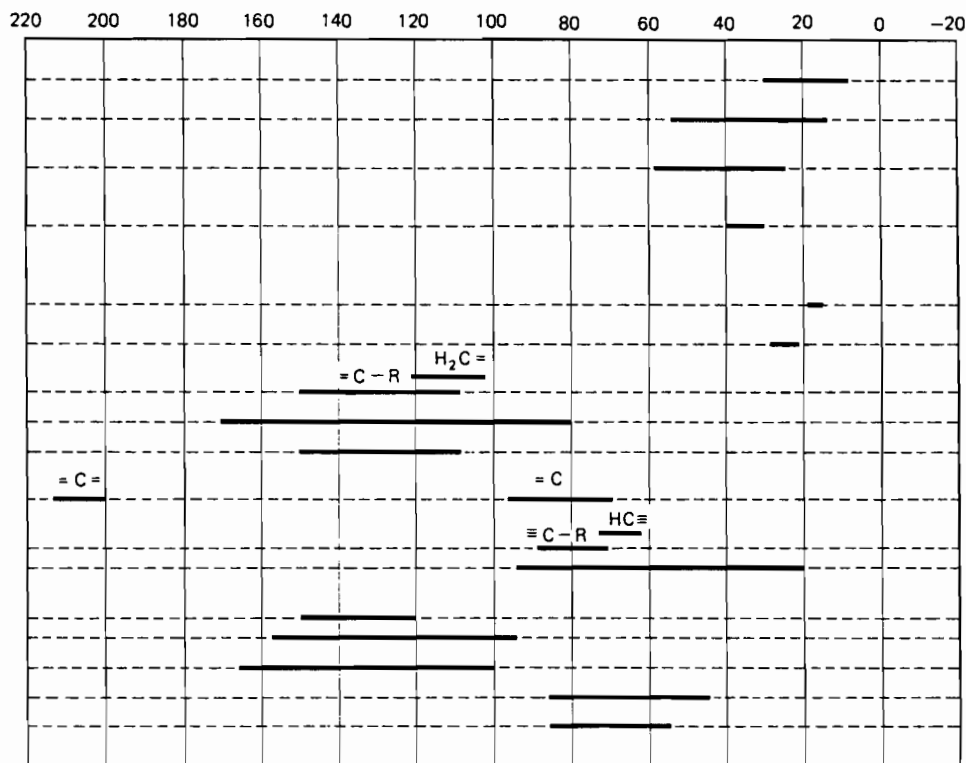
Ar - R

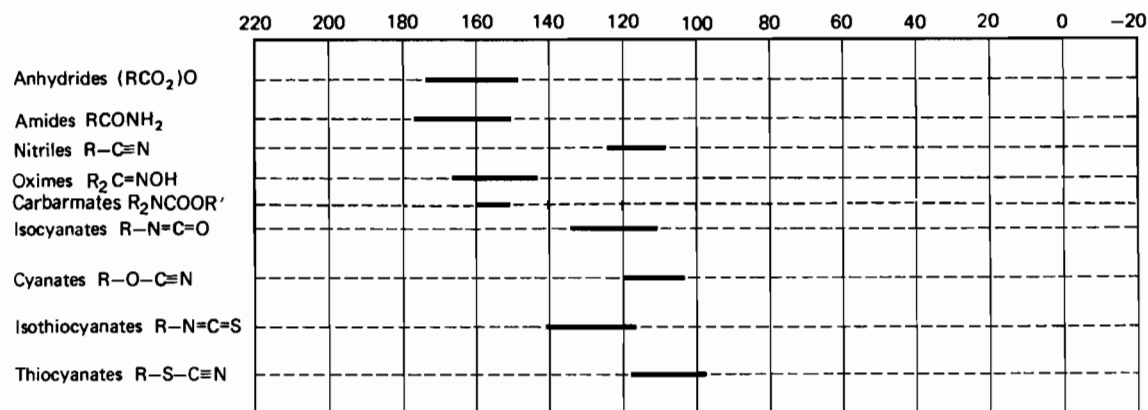
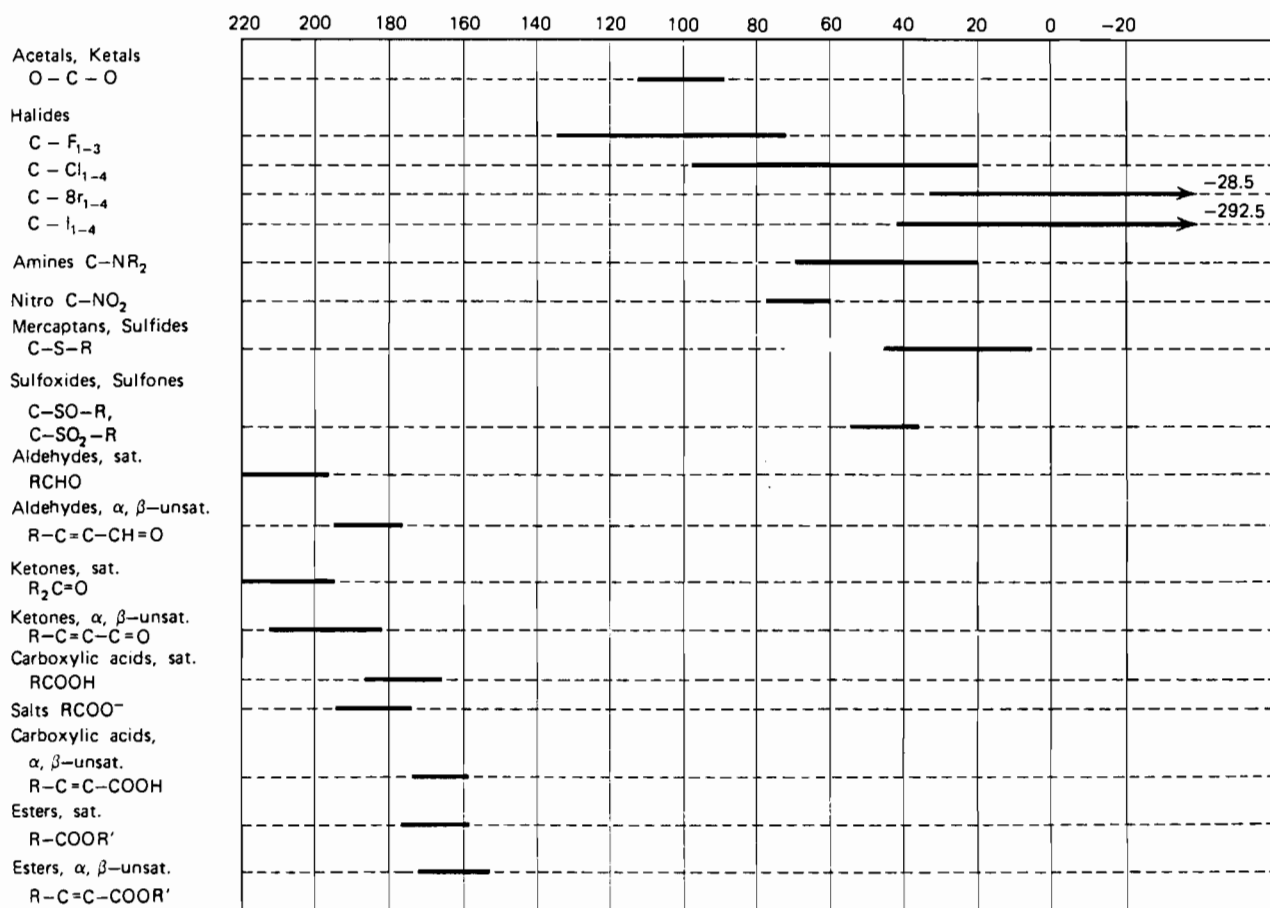
Ar - Y

Heteroaromatics

Alcohols C - OH

Ethers C - O - C



APPENDIX C (Continued)

APPENDIX D ^{13}C NMR DATA FOR SEVERAL NATURAL PRODUCTS (δ)