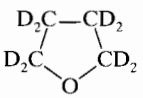
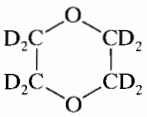
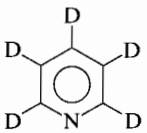
APPENDIX A THE ^{13}C CHEMICAL SHIFTS, COUPLINGS, AND MULTIPLICITIES OF COMMON NMR SOLVENTS

Structure	Name	δ(ppm)	J_{C-D}(Hz)	Multiplicity[a]
$CDCl_3$	Chloroform-d_1	77.0	32	Triplet
CD_3OD	Methanol-d_4	49.0	21.5	Septet
CD_3SOCD_3	DMSO-d_6	39.7	21	Septet
$DCON(CD_3)_2$	DMF-d_7	30.1	21	Septet
		35.2	21	Septet
		167.7	30	Triplet
C_6D_6	Benzene-d_6	128.0	24	Triplet
	THF-d_8	25.2	20.5	Quintet
		67.4	22	Quintet
	Dioxane-d_8	66.5	22	Quintet
	Pyridine-d_5	123.5 (C-3,5)	25	Triplet
		135.5 (C-4)	24.5	Triplet
		149.2 (C-2,6)	27.5	Triplet
CD_3CCD_3	Acetone-d_6	29.8 (methyl)	20	Septet
		206.5 (carbonyl)	<1	Septet[b]
CD_3CN	Acetonitrile-d_3	1.3 (methyl)	32	Septet
		118.2 (CN)	<1	Septet[b]
CD_3NO_2	Nitromethane-d_3	60.5	23.5	Septet
CD_3CD_2OD	Ethanol-d_6	15.8 (C-2)	19.5	Septet
		55.4 (C-1)	22	Quintet
$(CD_3CD_2)_2O$	Ether-d_{10}	13.4 (C-2)	19	Septet
		64.3 (C-1)	21	Quintet
$[(CD_3)_2N]_3P{=}O$	HMPA-d_{18}	35.8	21	Septet
CD_3CO_2D	Acetic acid-d_4	20.2 (C-2)	20	Septet
		178.4 (C-1)	<1	Septet[b]
CD_2Cl_2	Dichloromethane-d_2 (Methylene chloride-d_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.

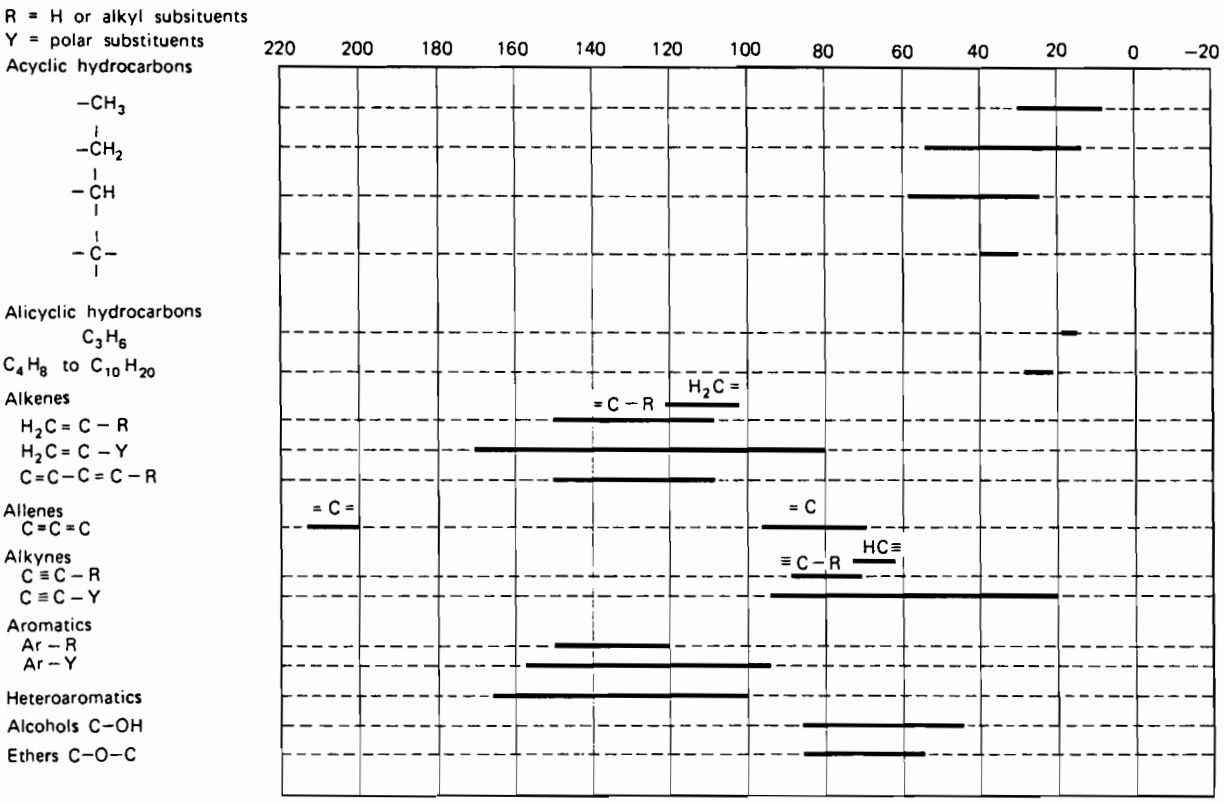
APPENDIX B ^{13}C CHEMICAL SHIFTS of COMMON LABORATORY SOLVENTS as TRACE IMPURITIES

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16 ± 0.06	29.84 ± 0.01 206.26 ± 0.13	39.52 ± 0.06	128.06 ± 0.02	1.32 ± 0.02 118.26 ± 0.02	49.00 ± 0.01	
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
tert-butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91	30.29
tert-butyl methyl	OCH_3	49.45	49.35	48.70	49.19	49.52	49.66	49.37
ether	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH_3Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88	66.42
diglyme	CH_3	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH_3	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH_2	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH_2CH_3	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	

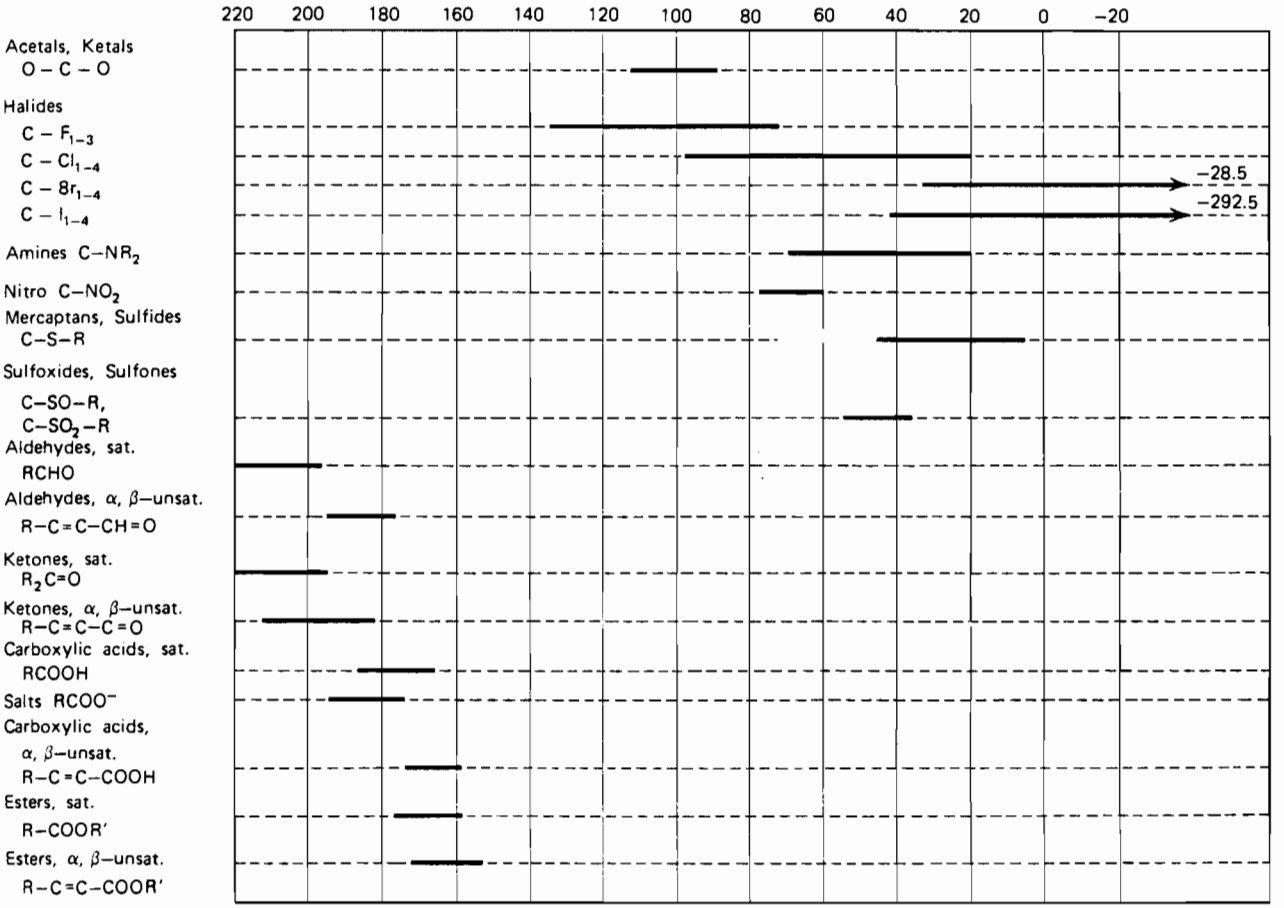
APPENDIX B *(Continued)*

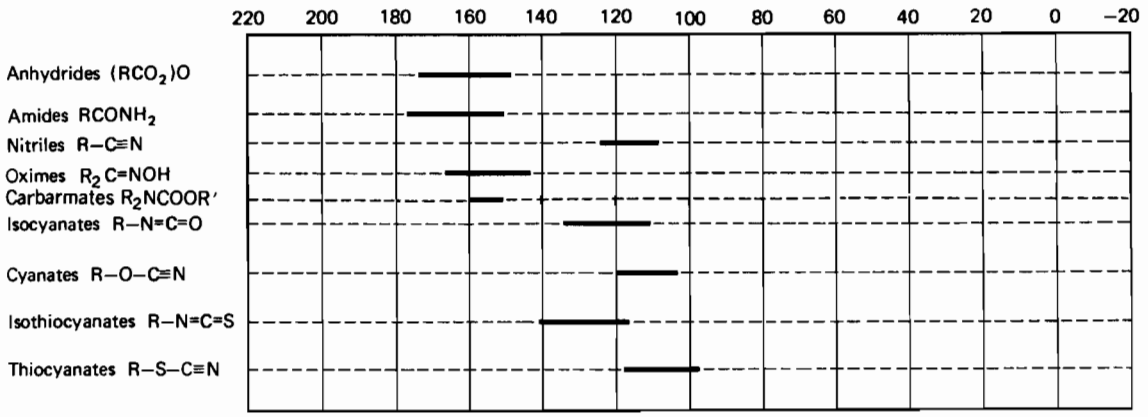
n-hexane	CH_3	14.14	14.34	13.88	14.32	14.43	14.45	
	$CH_2(2)$	22.70	23.28	22.05	23.04	23.40	23.68	
	$CH_2(3)$	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA	CH_3	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86	49.50
nitromethane	CH_3	62.50	63.21	63.28	61.16	63.66	63.08	63.22
n-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_2O	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*)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(*o*)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(*m*)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(*p*)	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 ^{13}C CORRELATION CHART FOR CHEMICAL CLASSES

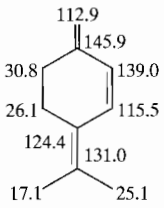


APPENDIX C *(Continued)*

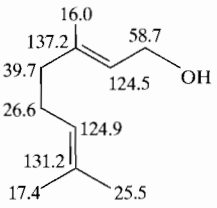




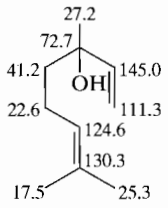
APPENDIX D ^{13}C NMR DATA FOR SEVERAL NATURAL PRODUCTS (δ)



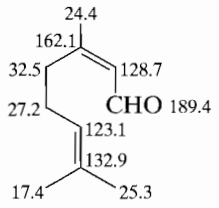
Myrcene



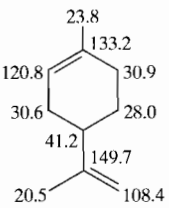
Geraniol



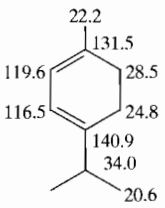
Linalool



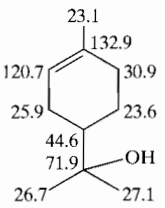
cis-Citral
(Neral, Citral b)



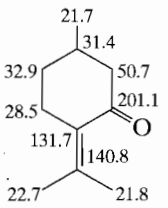
Limonene



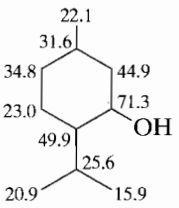
α-Terpinene



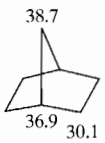
α-Terpineol



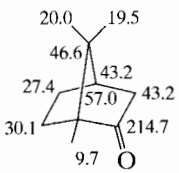
Pulegone



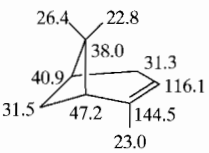
Menthol



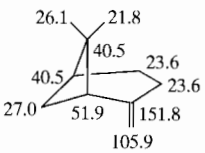
Norbornane



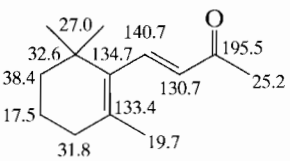
Camphor



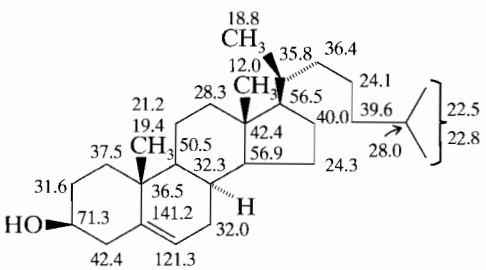
α-Pinene



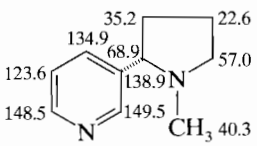
β-Pinene



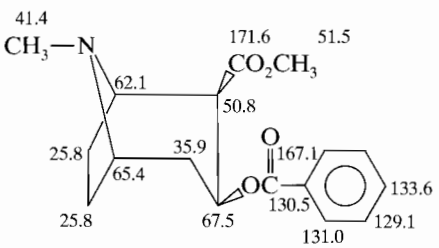
β-Ionone



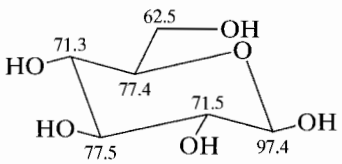
Cholesterol



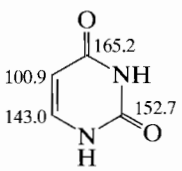
Nicotine



Cocaine



β-D-Glucose



Uracil