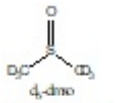
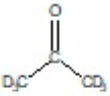
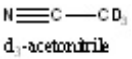
September 2019

Appendix V: NMR data of some common solvents:

These data are taken from Gottlieb, H.E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.*, **1997**, *62*, 7512.

Table 1: ^{1}H NMR Data

	Proton	**mult, J(Hz)**	**$CDCl_3$**  d-chloroform	**$(CD_3)_2SO$**  d_6-dmso d_6-dimethylsulfoxide	**C_6D_6**  d_6-benzene	**D_2O**  d_2-water	**$(CD_3)_2CO$**  d_6-acetone	**CD_3CN**  d_3-acetonitrile
solvent residual peak (mono-protonated)			7.24	2.5	7.16	4.8	2.05	1.94
water traces			1.56	3.33 H_2O 3.30 HOD	0.4	-	2.84 H_2O 2.81 HOD	2.13
acetic acid	CH_3	s	2.1	1.91	1.55	2.08	1.96	1.96
acetone	CH_3	s	2.17	2.09	1.55	2.22	2.09	2.08
acetonitrile	CH_3	s	2.1	2.07	1.55	2.06	2.05	1.96
benzene	CH	s	7.36	7.37	7.15		7.36	7.37
tert-butyl alcohol	CH_3 OH	s s	1.28	1.11 4.19	1.05 1.55	1.24	1.18	1.16 2.18
chloroform	CH	s	7.26	8.32	6.15		8.02	7.58
cyclohexane	CH_2	s	1.43	1.4	1.4		1.43	1.44
1,2-dichloroethane	CH_2	s	3.73	3.9	2.9		3.87	3.81
dichloromethane	CH_2	s	5.3	5.76	4.27		5.63	5.44
diethyl ether	CH_3 CH_2	t,7 q,7	1.21 3.48	1.09 3.38	1.11 3.26	1.17 3.56	1.11 3.41	1.12 3.42
diglyme	CH_2 CH_2 OCH_3	m m s	3.65 3.57 3.39	3.51 3.38 3.24	3.46 3.34 3.11	3.67 3.61 3.37	3.56 3.47 3.28	3.53 3.45 3.29
1,2-dimethoxyethane	CH_3 CH_2	s s	3.40 3.55	3.24 3.43	3.12 3.33	3.37 3.60	3.28 3.46	3.28 3.45
dimethylformamide	CH CH_3 CH_3	s s s	8.02 2.96 2.88	7.95 2.89 2.73	7.63 2.36 1.86	7.92 3.01 2.85	7.96 2.94 2.78	7.92 2.89 2.77

Appendix V - 2

	Proton	**mult, J(Hz)**	**$CDCl_3$**	**$(CD_3)_2SO$**	**C_6D_6**	**D_2O**	**$(CD_3)_2CO$**	**CD_3CN**
dimethyl sulfoxide	C*H*$_3$	s	2.62	2.54	1.68	2.71	2.52	2.50
ethanol	C*H*$_3$ C*H*$_2$ O*H*	t,7 q,7 s	1.25 3.72 1.32	1.06 3.44 4.63	0.96 3.34	1.17 3.65	1.12 3.57	1.12 3.54
ethyl acetate	C*H*$_3$CO C*H*$_2$CH$_3$ CH$_2$C*H*$_3$	s q,7 t,7	2.05 4.12 1.26	1.99 4.03 1.17	1.65 3.89 0.92	2.07 4.14 1.24	1.97 4.05 1.20	1.97 4.06 1.20
n-hexane	C*H*$_3$ C*H*$_2$	t m	0.88 1.26	0.86 1.25	0.89 1.24		0.88 1.28	0.89 1.28
methanol	C*H*$_3$ O*H*	s s	3.49 1.09	3.16 4.01	3.07	3.34	3.31 3.12	3.28 2.16
n-pentane	C*H*$_3$ C*H*$_2$	t,7 m	0.88 1.27	0.86 1.27	0.87 1.23		0.88 1.27	0.89 1.29
2-propanol	C*H*$_3$ C*H*	d,6 sep,6	1.22 4.04	1.04 3.78	0.95 3.67	1.17 4.02	1.10 3.90	1.09 3.87
pyridine	C*H*(2) C*H*(3) C*H*(4)	m m m	8.62 7.29 7.68	8.58 7.39 7.79	8.53 6.66 6.98	8.52 7.45 7.87	8.58 7.35 7.76	8.57 7.33 7.73
silicon grease	C*H*$_3$	s	0.07		0.29		0.13	0.08
tetrahydrofuran	C*H*$_2$ C*H*$_2$O	m m	1.85 3.76	1.76 3.60	1.40 3.57	1.88 3.74	1.79 3.63	1.80 3.64
toluene	C*H*$_3$ C*H*(*o/p*) C*H(m)*	s m m	2.36 7.17 7.25	2.30 7.18 7.25	2.11 7.02 7.13		2.32 7.1/7.2 7.1/7.2	2.33 7.1-7.3 7.1-7.3
triethylamine	C*H*$_3$ C*H*$_2$	t,7 q,7	1.03 2.53	0.93 2.43	0.96 2.40	0.99 2.57	0.96 2.45	0.96 2.45

Table 2: ^{13}C NMR Data

	Carbon	**$CDCl_3$**	**$(CD_3)_2SO$**	**C_6D_6**	**D_2O**	**$(CD_3)_2CO$**	**CD_3CN**
solvent peak		77.16 +/- 0.06	39.52 +/- 0.06	128.06 +/- 0.02	-	29.84 +/-0.01 206.26 +/-0.13	1.32 +/-0.02 118.26 +/-0.02
acetic acid	*C*O *C*H_3	175.99 20.81	171.93 20.95	175.82 20.37	177.21 21.03	172.31 20.51	173.21 20.73
acetone	*C*O *C*H_3	207.07 30.92	206.31 30.56	204.43 30.14	215.94 30.89	205.87 30.60	207.43 30.91
acetonitrile	*C*N *C*H_3	116.43 1.89	117.91 1.03	116.02 0.20	119.68 1.47	117.60 1.12	118.26 1.79
benzene	*C*H	128.37	128.3	128.62		129.15	129.32
tert-butyl alcohol	*C* *C*H_3	69.15 31.25	66.88 30.38	68.19 30.47	70.36 30.29	68.13 30.72	69.40 30.91
chloroform	*C*H	77.36	79.16	77.79		79.19	79.17
cyclohexane	*C*H_2	26.94	26.33	27.23		27.51	27.63
1,2-dichloroethane	*C*H_2	43.5	45.02	43.59		45.25	45.54
dichloromethane	*C*H_2	53.52	54.84	53.46		54.95	55.32
diethyl ether	*C*H_3 *C*H_2	15.20 65.91	15.12 62.05	15.46 65.94	14.77 66.42	15.78 66.12	15.63 66.32
diglyme	*C*H_3 *C*H_2 *C*H_2	59.01 70.51 71.90	57.98 69.54 71.25	58.66 70.87 72.35	58.67 70.05 71.63	58.77 71.03 72.63	58.90 70.99 72.63
1,2-dimethoxyethane	*C*H_3 *C*H_2	59.08 71.84	58.01 17.07 ?	58.68 72.21	58.67 71.49	58.45 72.47	58.89 72.47
dimethylformamide	*C*H *C*H_3 *C*H_3	162.62 36.50 31.45	162.29 35.73 30.73	162.13 35.25 30.72	165.53 37.54 32.03	162.79 36.15 31.03	163.31 36.57 31.32
dimethyl sulfoxide	*C*H_3	40.76	40.45	40.03	39.39	41.23	41.31
ethanol	*C*H_3 *C*H_2	18.41 58.28	18.51 56.07	18.72 57.86	17.47 58.05	18.89 57.72	18.80 57.96
ethyl acetate	*C*H_3CO *C*O *C*H_2 *C*H_3	21.04 171.36 60.49 14.19	20.68 170.31 59.74 14.40	20.56 170.44 60.21 14.19	21.15 175.26 62.32 13.92	20.83 170.96 60.56 14.50	21.16 171.68 60.98 14.54

	Carbon	**$CDCl_3$**	**$(CD_3)_2SO$**	**C_6D_6**	**D_2O**	**$(CD_3)_2CO$**	**CD_3CN**
n-hexane	*C*H_3 *C*H_2(2) *C*H_2(3)	14.14 22.70 31.64	13.88 22.05 30.95	14.32 23.04 31.96		14.34 23.28 32.30	14.43 23.40 32.36
methanol	*C*H_3	50.41	48.59	49.97	49.5	49.77	49.90
n-pentane	*C*H_3 *C*H_2(2) *C*H_2(3)	14.08 22.38 34.16	13.28 21.70 33.48	14.25 22.72 34.45		14.29 22.98 34.83	14.37 23.08 34.89
2-propanol	*C*H_3 *C*H	25.14 64.50	25.43 64.92	25.18 64.23	24.38 64.88	25.67 63.85	25.55 64.30
pyridine	*C*H(2) *C*H(3) *C*H(4)	149.90 123.75 135.96	149.58 123.84 136.05	150.27 123.58 135.28	149.18 125.12 138.27	150.67 124.57 136.56	150.76 127.76 136.89
silicon grease	*C*H_3	1.04		1.38		1.4	
tetrahydrofuran	*C*H_2 *C*H_2O	25.62 67.97	25.14 67.03	25.72 67.80	25.67 68.68	26.15 68.07	26.27 68.33
toluene	*C*H_3 *C*(*i*) *C*H(*o*) *C*H(*m*) *C*H(*p*)	21.46 137.89 129.07 128.26 125.33	20.99 137.35 128.88 128.18 125.29	21.10 137.91 129.33 128.56 125.68		21.46 138.48 129.76 129.03 126.12	21.50 138.90 129.94 126.28
triethylamine	*C*H_3 *C*H_2	11.61 46.25	11.74 45.74	12.35 46.77	9.07 47.19	12.49 47.07	12.38 47.10