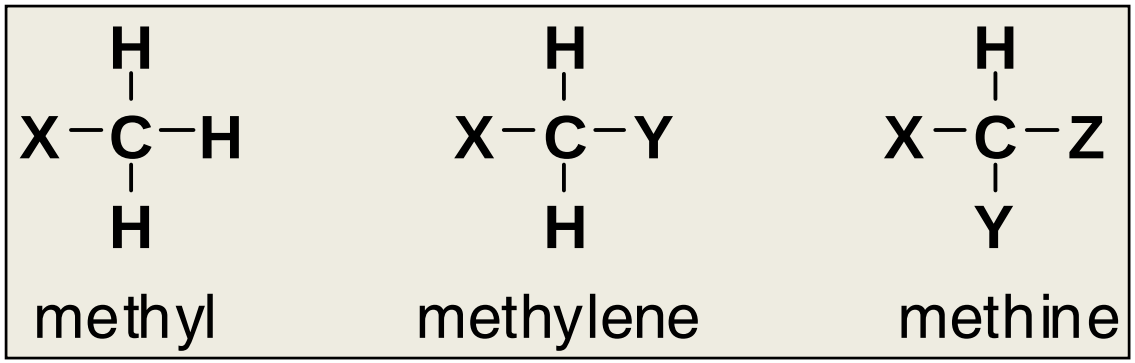
Shoolery Tables

- After years of collective observation of ^{1}H and ^{13}C NMR it is possible to predict chemical shift to a fair precision using Shoolery Tables

- These tables use a base value for ^{1}H and ^{13}C chemical shift to which are added adjustment increments for each group on the carbon atom



Shoolery Values for Methylene

X or Y	Substituent Constant
-H	0.34
-CH_3	0.68
-C—C	1.32
-C≡C-	1.44
-Ph	1.83
-CF_2-	1.12
-CF_3	1.14
-F	3.30
-Cl	2.53
-Br	2.33
-I	2.19
-OH	2.56
-OR	2.36
-OPh	2.94

X or Y	Substituent Constant
-OC(=O)OR	3.01
-OC(=O)Ph	3.27
-C(=O)R	1.50
-C(=O)Ph	1.90
-C(=O)OR	1.46
-C(=O)NR_2 or H_2	1.47
-C≡N	1.59
-NR_2 or H_2	1.57
-NHPh	2.04
-NHC(=O)R	2.27
-N_3	1.97
-NO_2	3.36
-SR or H	1.64
-OSO_2R	3.13

Shoolery Values for Methine

X ,Y or Z	Substituent Constant
-F	1.59
-Cl	1.56
-Br	1.53
-NO_2	1.84
-NR_2 or H_2	0.64
-NH_3^+	1.34
-NHC(=O)R	1.80
-OH	1.14
-OR	1.14
-C(=O)OR	2.07
-OPh	1.79

X, Y or Z	Substituent Constant
-OC(=O)OR	0.47
-C(=O)R	0.47
-C(=O)Ph	1.22
-C≡N	0.66
-$C(=O)NH_2$	0.60
-SR or H	0.61
-OSO_2R	0.94
-C≡C-	0.79
-C=C	0.46
-Ph	0.99

Shoolery Tables

- For methyl—use methylene formula and table using the –H value

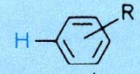
- For methylene—use a base value of 0.23 and add the two substituent constants for X and Y
  In 92% of cases experimental is within 0.2 ppm

- For methine—use a base value of 2.50 and add the three substituent constants for X, Y and Z
  Error similar to methylene

Shoolery Tables

- Work for aromatics as well (.pdf posted)

Increment system for the estimation of chemical shifts of benzene protons

$\delta = 7.26 = \Sigma I$ 			
Substituent	I_{ortho}	I_{meta}	I_{para}
—H	0	0	0
—CH_3	− 0.18	− 0.10	− 0.20
—CH_2CH_3	− 0.15	− 0.06	− 0.18
—$CH(CH_3)_2$	− 0.13	− 0.08	− 0.18
—$C(CH_3)_3$	0.02	− 0.09	− 0.22
—CH_2Cl	0.00	0.01	0.00
—CH_2OH	− 0.07	− 0.07	− 0.07
—CH_2NH_2	0.01	0.01	0.01
—$CH{=}CH_2$	0.06	− 0.03	− 0.10
—$C{\equiv}CH$	0.15	− 0.02	− 0.01
—C_6H_5	0.30	0.12	0.10
—CHO	0.56	0.22	0.29
—CO—CH_3	0.62	0.14	0.21
—CO—CH_2—CH_3	0.63	0.13	0.20
—CO—C_6H_5	0.47	0.13	0.22
—COOH	0.85	0.18	0.25
—$COOCH_3$	0.71	0.11	0.21
—CO—O—C_6H_5	0.90	0.17	0.27
—CO—NH_2	0.61	0.10	0.17
—COCl	0.84	0.20	0.36
—CN	0.36	0.18	0.28
—NH_2	− 0.75	− 0.25	− 0.65
—NH—CH_3	− 0.80	− 0.22	− 0.68
—$N(CH_3)_2$	− 0.66	− 0.18	− 0.67
—$N(CH_3)_3I^-$	0.69	0.36	0.31
—NH—$COCH_3$	0.12	− 0.07	− 0.28
—NO	0.58	0.31	0.37
—NO_2	0.95	0.26	0.38
—SH	− 0.08	− 0.16	− 0.22
—SCH_3	− 0.08	− 0.10	− 0.24
—S—C_6H_5	0.06	− 0.09	− 0.15
—SO_2—OH	0.64	0.26	0.36
—SO_2—NH_2	0.66	0.26	0.36
—OH	− 0.56	− 0.12	− 0.45
—OCH_3	− 0.48	− 0.09	− 0.44
—OCH_2—CH_3	− 0.46	− 0.10	− 0.43
—O—C_6H_5	− 0.29	− 0.05	− 0.23
—O—CO—CH_3	− 0.25	0.03	− 0.13
—O—CO—C_6H_5	− 0.09	0.09	− 0.08
—F	− 0.26	0.00	− 0.20
—Cl	0.03	− 0.02	− 0.09
—Br	0.18	− 0.08	− 0.04
—I	0.39	− 0.21	− 0.03