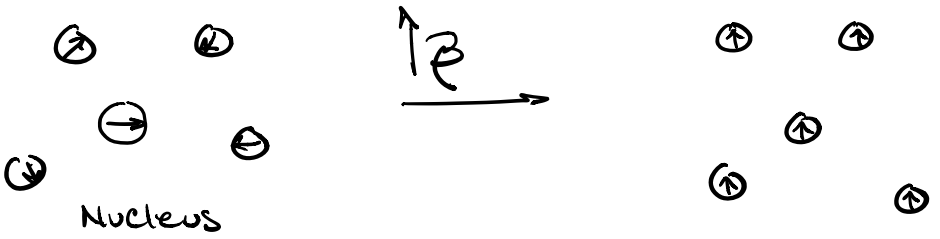
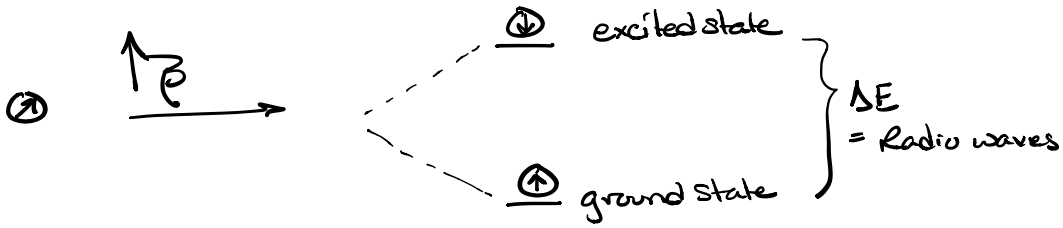
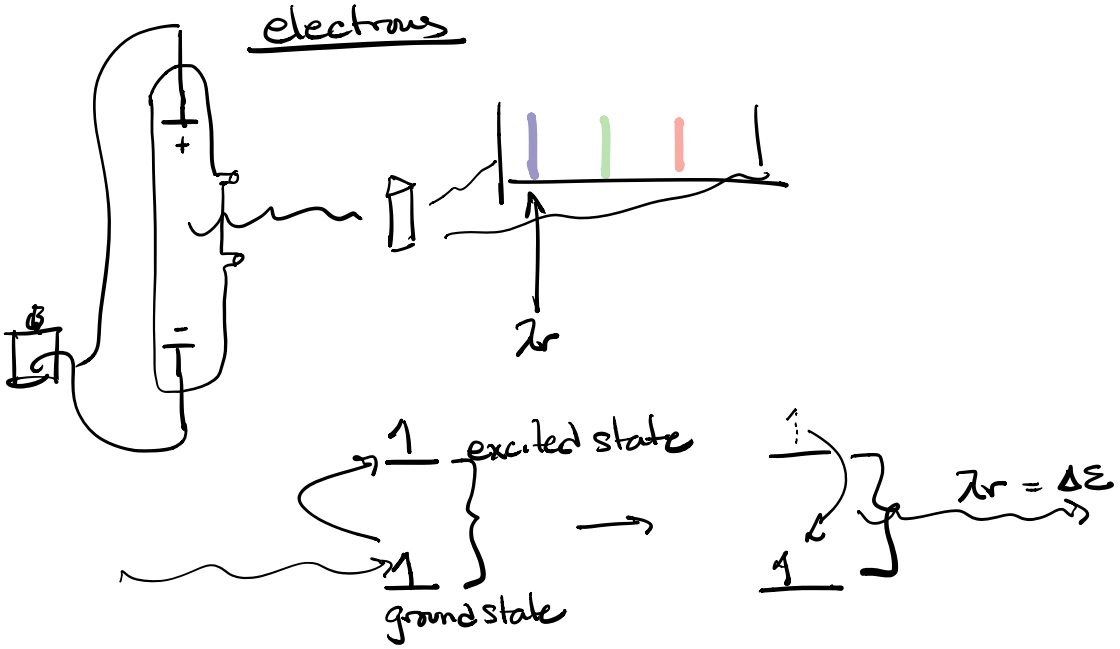
Spectroscopy

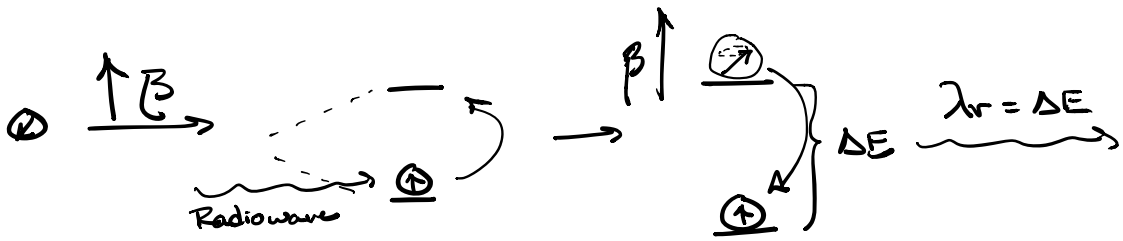
NMR - Nuclear Magnetic Resonance



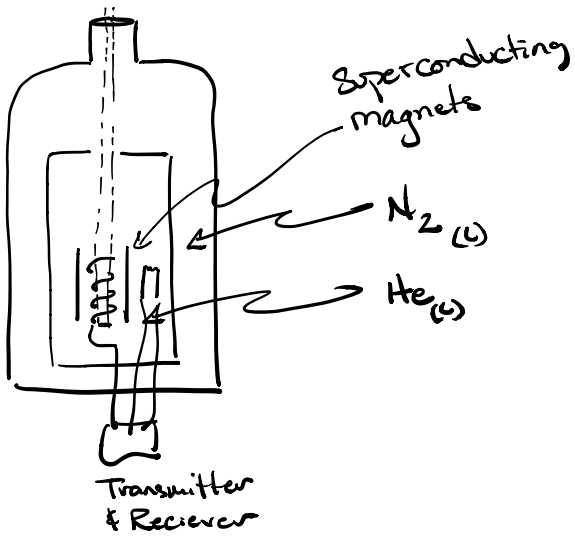
↑ spin of the nucleus B = magnetic field







NMR



NMR only works on odd spin nuclei

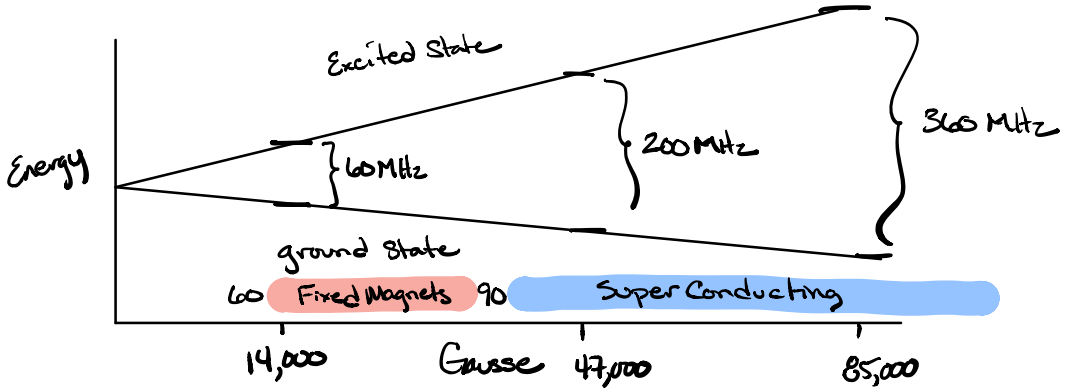
$I = 1/2, 3/2, \ldots$

	I	
→ ^{1}H	1/2	99.9850%
^{2}H	1	0.0150%
^{12}C	1	98.900%
→ ^{13}C	1/2	1.100%

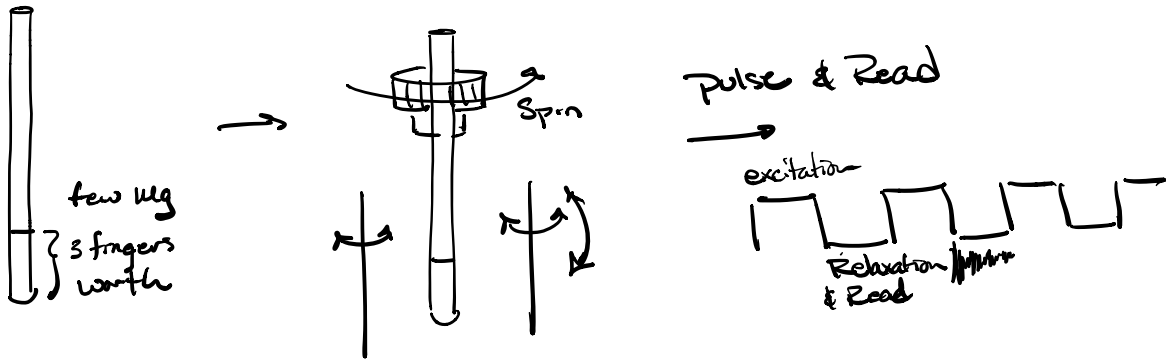
	I	
^{14}N	1	99.634%
^{15}N	1/2	0.3660%

The difference in Energy between ground state & excited State is very small $\propto$ to Strength of $\vec{B}$ field

^{1}HNMR

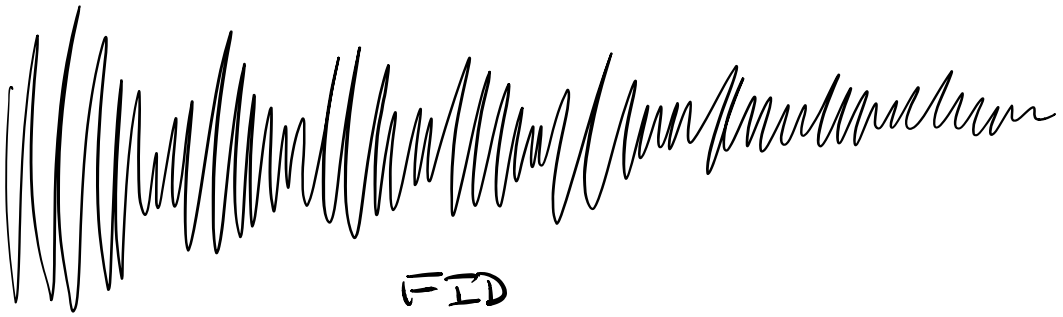


NMR Experiment



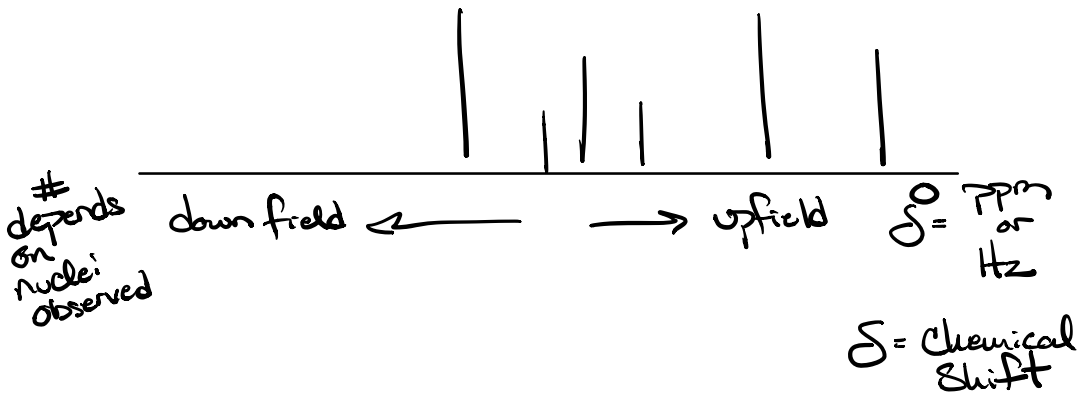
Shimming
→ Homogeneous magnetic field

Output Free Induction Decay



FID

↓ Fourier Transformation



δ = Chemical Shift

^{1}H-NMR 14 – 0 ppm

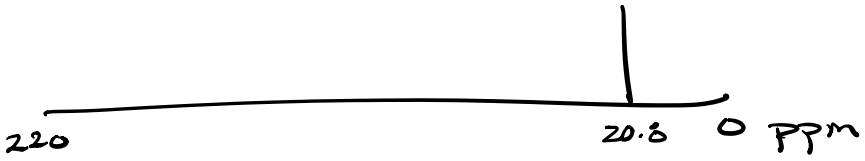
^{13}C-NMR 220 – 0 ppm

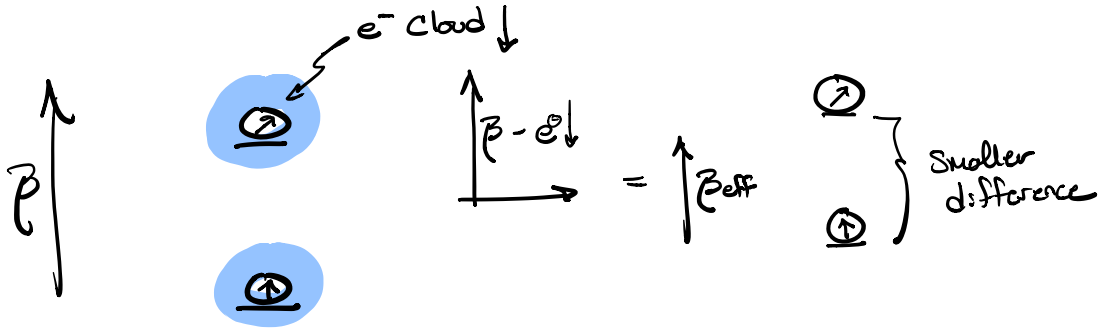
$$\delta = \frac{\nu_{sample} - \nu_{Ref}}{\nu_{applied}} \times 10^{6} = ppm$$

Ex

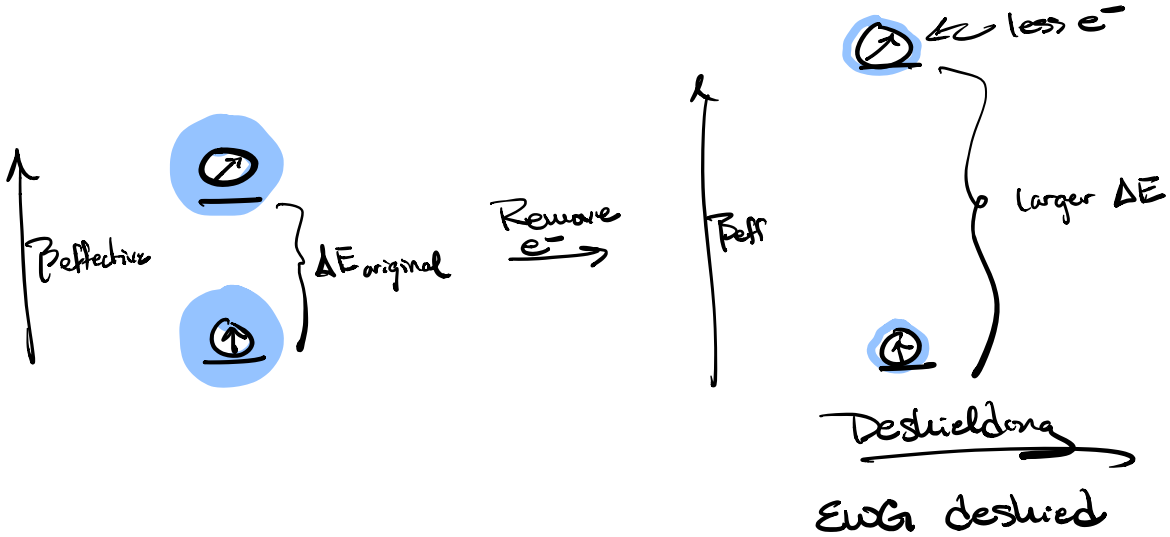
50 MHz ^{13}C & Signal 1040 Hz down field

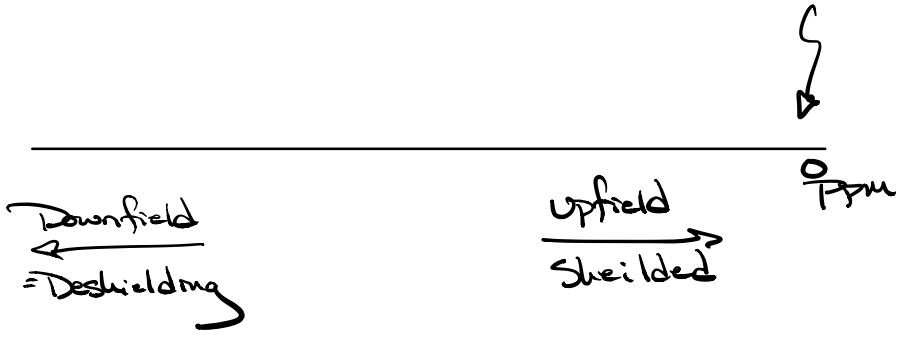
$$\delta = \frac{1040 - 0}{50 \times 10^6} \times 10^6 = 20.8 \text{ ppm}$$

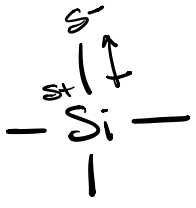




if we remove outter e⁻ density



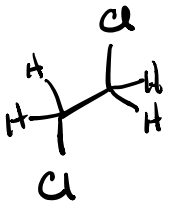




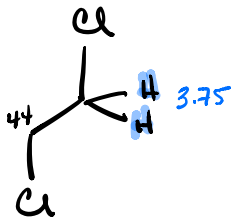
Tetramethyl Silane

TMS

Si EDG

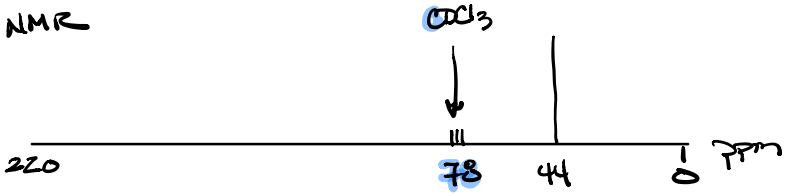


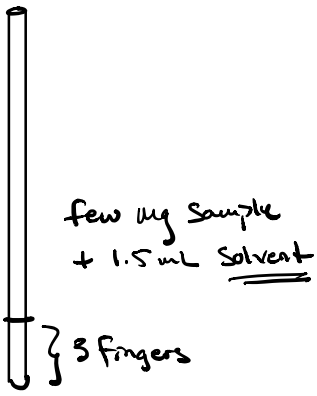
1,2-dichloroethane



^{1}H-NMR

^{13}C-NMR





Deuterated NMR Solvents

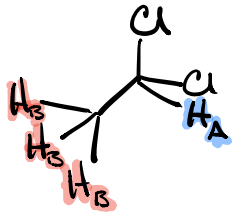
$CDCl_3$ D ?

^{1}H ^{2}H = D

proton deuterium

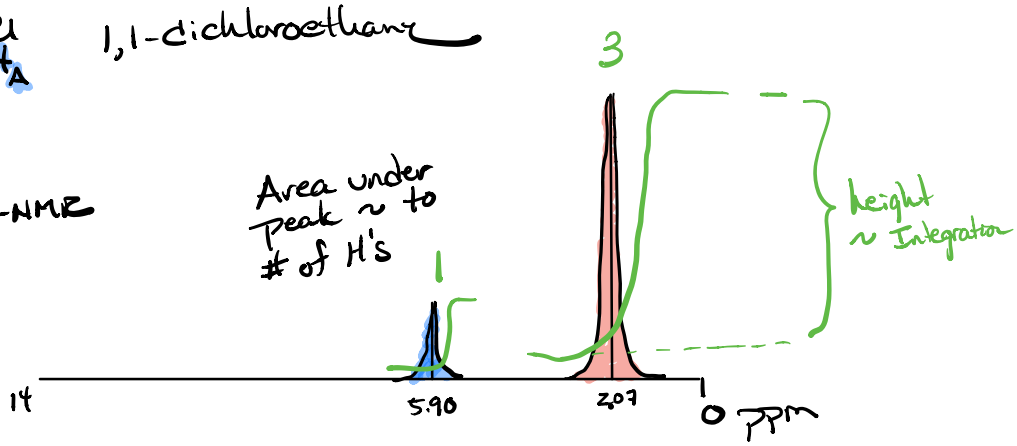
I = ½ I = 1

CD_3OD

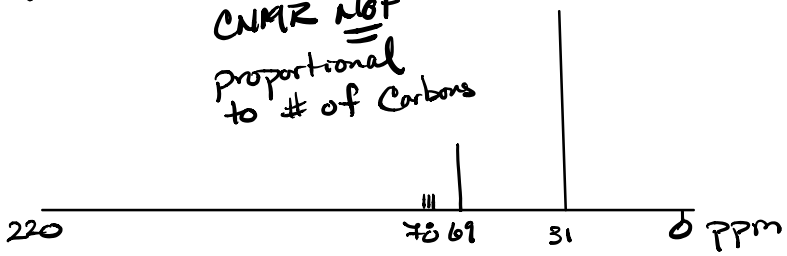


1,1-dichloroethane

^{1}H-NMR

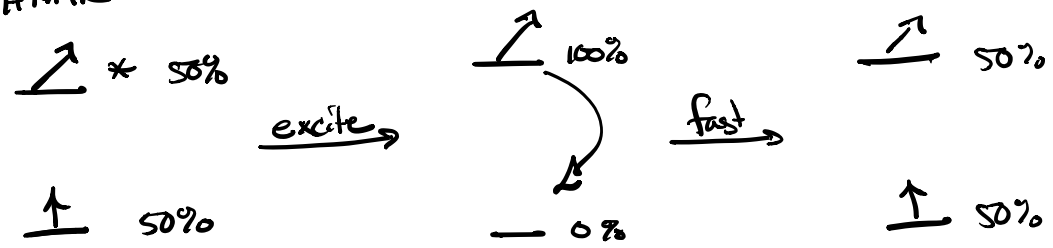


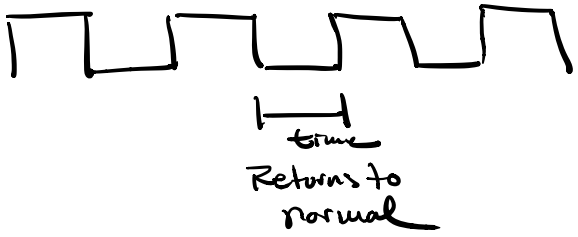
^{13}C-NMR

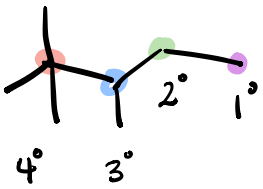


protons relax very quickly

HNMR



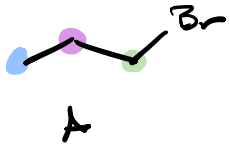




Relaxation Rates differ $1° >> 2° > 3° > 4°$

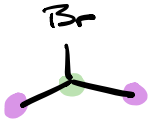
↑ Extremely Slow

For Equal #'s of Carbons



A

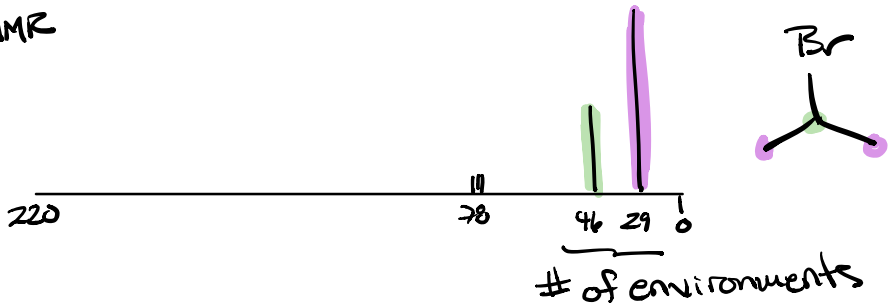
3 Signals
= 3 Environments



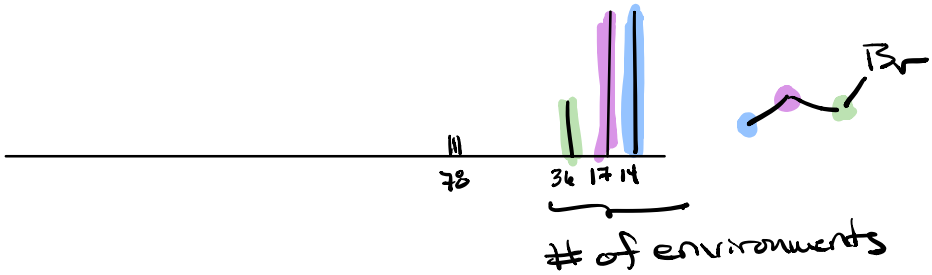
B

2 Signals = 2 Chemical Environments

^{13}CNMR



^{13}CNMR



$$\delta = \frac{\nu_{sample} - \nu_{ref}}{\nu_{applied}} \times 10^6$$