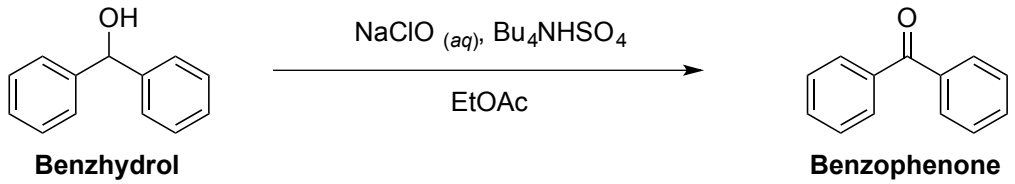
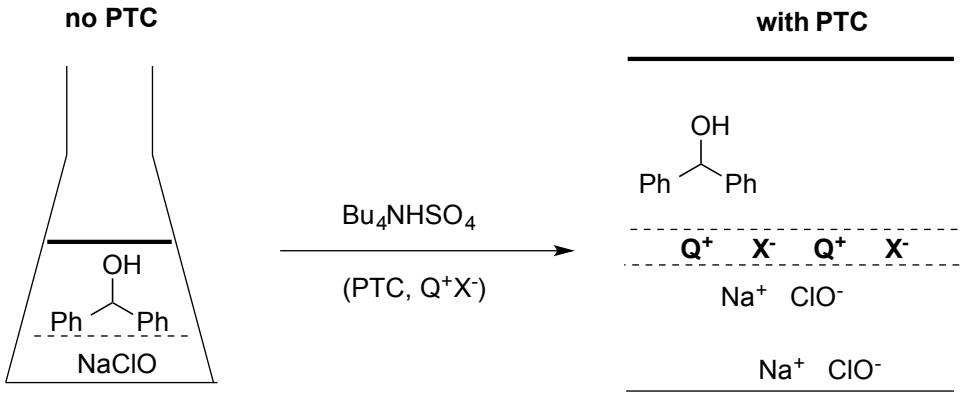
CHEM 8M, Experiment 3 – Oxidation of Benzhydrol

- Reactions using Phase Transfer Catalysts (PTC)
- TLC, IR, and ^{1}H NMR Analysis of Benzhydrol & Benzophenone

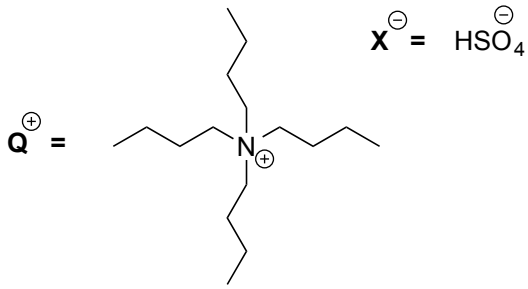
Oxidation of Benzhydrol with Bleach using Phase Transfer Catalyst



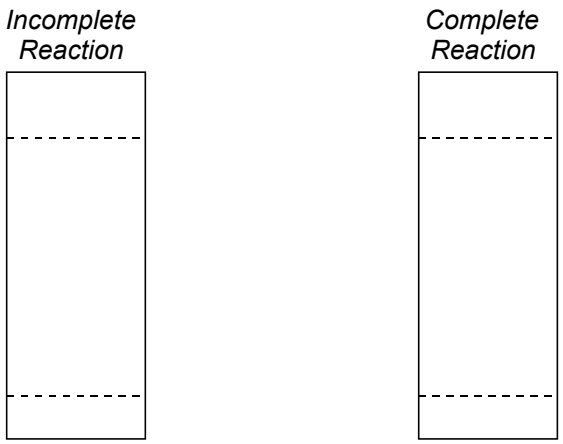
Phase Transfer Catalysis (PTC)



Bu_4NHSO_4 = tetrabutyl ammonium sulfate



Monitoring Reaction Progress by TLC



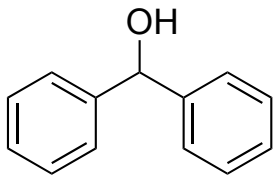
Reaction Work-up: remove AQ, wash with brine then water, dry, filter, rota-vap

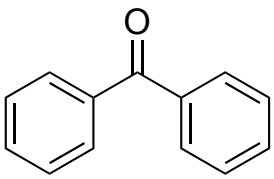
IR Analysis

^{1}H NMR Analysis = assign each set of protons on structure to signal on spectrum

Predict spectrum

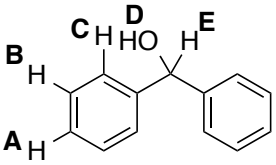
1. Look for symmetry – **equivalent protons** and for asymmetry – **non-equivalent protons**



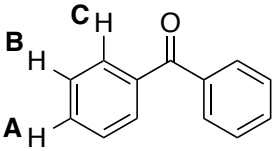


2. Integration: How many of each type of proton?

3. Identify **chemical shift ranges** in benzhydrol & benzophenone



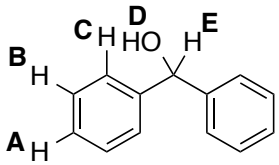
Benzhydrol



Benzophenone

4. Calculate **expected chemical shifts** using chemical shift correlation tables or online predictor tool

Table 3. ^{1}H NMR Analysis of Benzhydrol

	Signal	Integration (# of H's)	Expected Chemical Shift (ppm)	Observed Chemical Shift (ppm)
 **Benzhydrol**	**A**			
	B			
	C			
	D			
	E			

Correlate / assign to signals on given spectrum

- *Integration lines = Curves on or above peaks, height = relative ratio of H's*

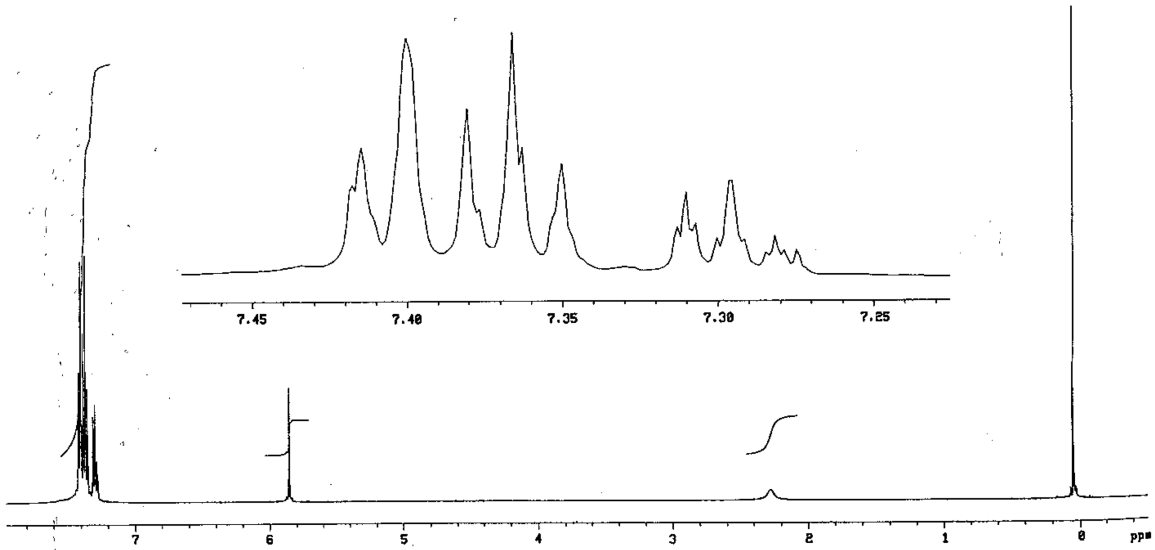
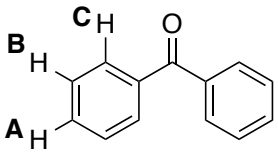


Figure 21.6 500-MHz ^{1}H-NMR spectrum of benzhydrol in $CDCl_3$.

Table 4. ^{1}H NMR Analysis of Benzophenone

 Benzophenone	Signal	Integration (# of H's)	Expected Chemical Shift (ppm)	Observed Chemical Shift (ppm)
	A'			
	B'			
	C'			

Correlate / assign to signals on given spectrum

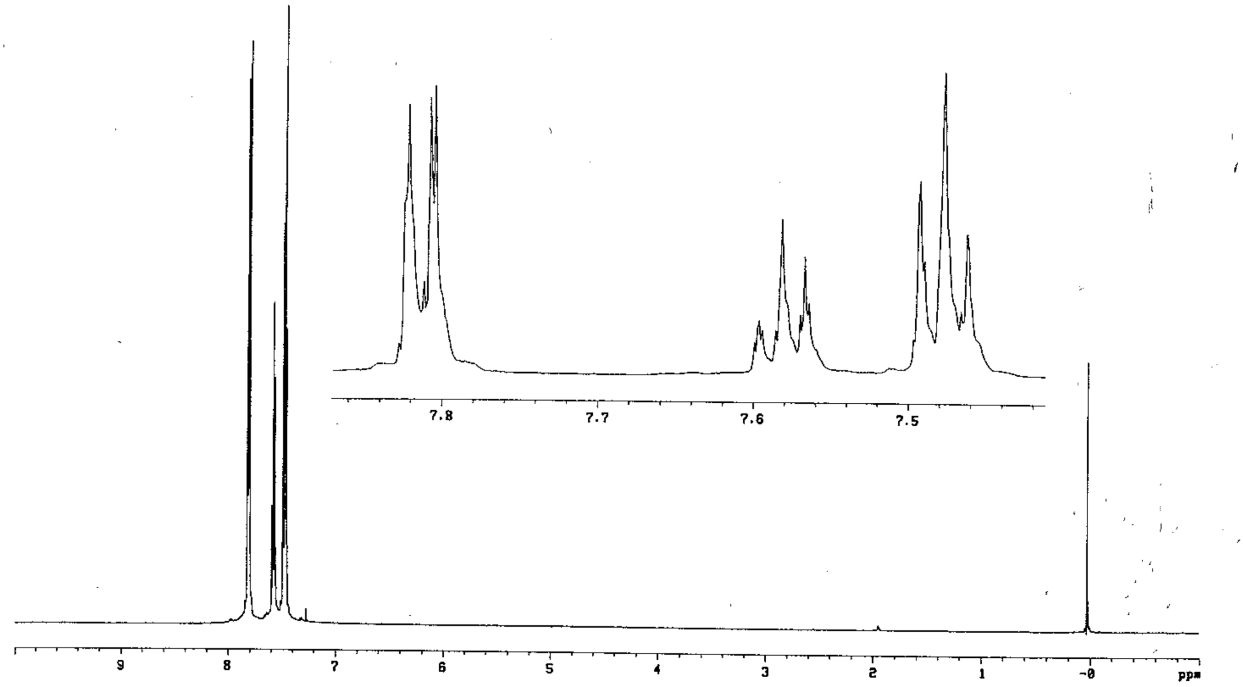


Figure 21.3 500-MHz ^{1}H-NMR spectrum of benzophenone in $CDCl_3$.

Supplemental Reading

Klein, D. "Organic Chemistry, 2nd Edition"; **Mohrig**, J. R.; *et. al*. "Techniques in Organic Chemistry, 4th Edition."
See also Exp 3 pre-lab videos on Canvas

Oxidation reactions	Klein 12.10
^{1}H NMR	Klein 15.1-6 or Mohrig Chapter 22.1-22.7
Extraction	Mohrig Chapter 10
TLC	Mohrig Chapter 18