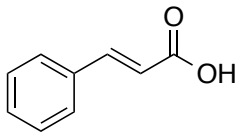
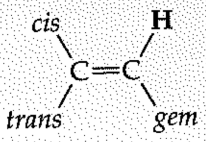
CHEM 110L, Lecture 3
Exp 2 – ^{1}H & ^{13}C NMR – *trans*-cinnamic acid
Exp 3 – Pseudoionones

^{1}H NMR of *trans*-Cinnamic Acid



Signal	Integration (#H's)	Splitting	Chemical Shift, Expected (ppm)	Chemical Shift, Observed (ppm)
A				
B				
C				
D				
E				
F				

TABLE 21.5 Additive Parameters for Predicting NMR Chemical Shifts of Vinyl Protons in $CDCl_3$[a]

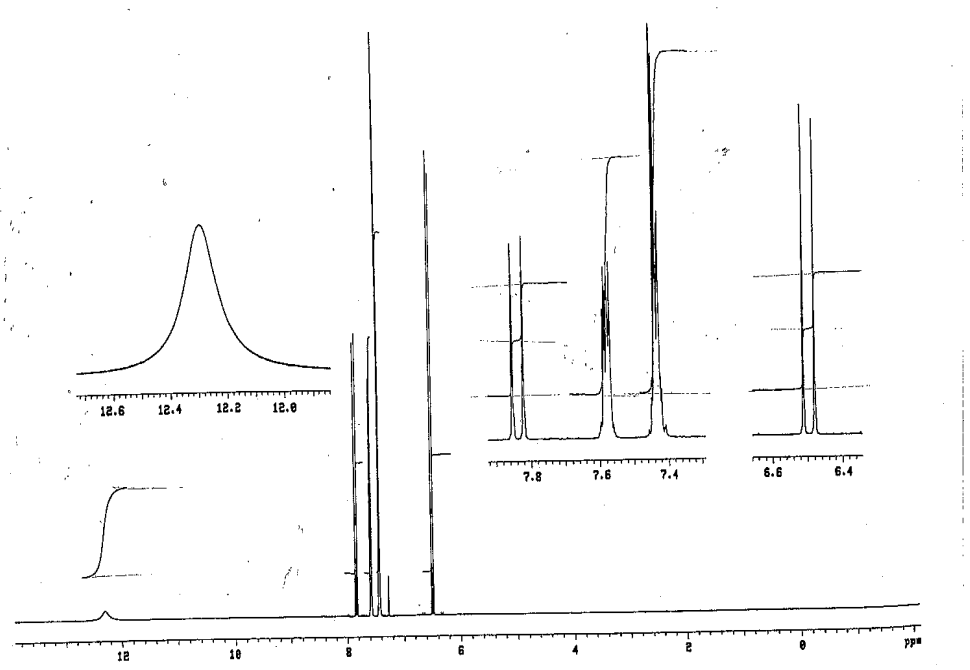


Base value 5.28 ppm

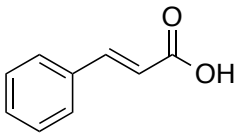
Group	*gem*	*cis*	*trans*
—R	0.45	−0.22	−0.28
—CH=CH_2	1.26	0.08	−0.01
—CH_2OH	0.64	−0.01	−0.02
—CH_2X (X=F, Cl, Br)	0.70	−0.11	−0.04
—(C=O)OH	0.97	1.41	0.71
—(C=O)OR	0.80	1.18	0.55
—(C=O)H	1.02	0.95	1.17
—(C=O)R	1.10	1.12	0.87
—(C=O)Ar	1.82	1.13	0.63
—Ar	1.38	0.36	−0.07
—Br	1.07	0.45	0.55
—Cl	1.08	0.18	0.13
—OR	1.22	−1.07	−1.21
—OAr	1.21	−0.60	−1.00
—O(C=O)R	2.11	−0.35	−0.64
—NH_2, —NHR, —NR_2	0.80	−1.26	1.21
—NH(C=O)R	2.08	−0.57	−0.72

a. There may be small differences in the chemical-shift values calculated from this table and those measured from individual spectra.

Literature spectra (Palleros text):



^{13}C NMR



Signal	Chemical Shift, Estimated	Chemical Shift, Observed
A'		
B'		
C'		
D'		
E'		
F'		
G'		

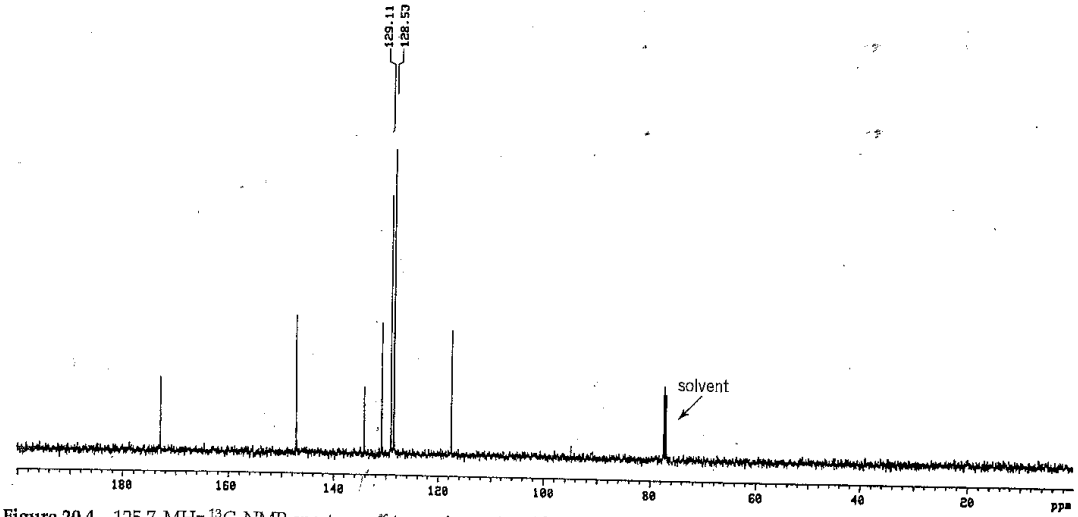
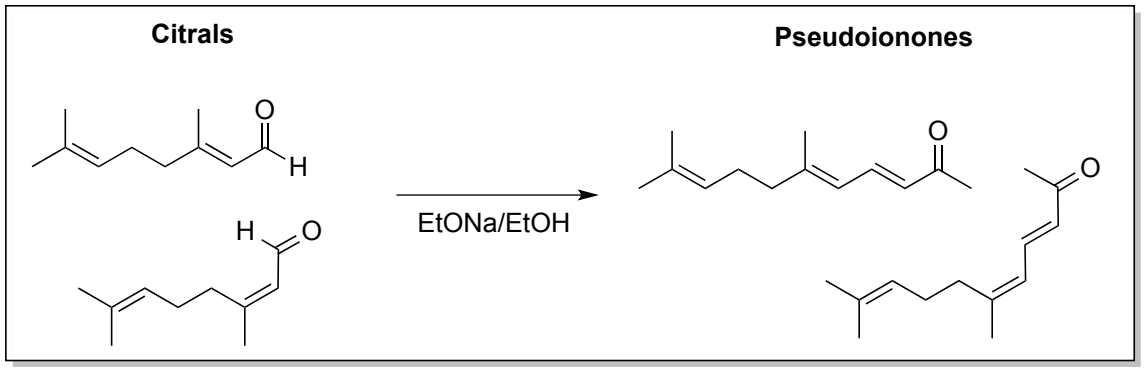


Figure 20.4 125.7-MHz ^{13}C-NMR spectrum of *trans*-cinnamic acid in $CDCl_3$.

Exp 3 – Two-Step Synthesis of Ionones

Step 1 (week 1)…



Aldol Condensation