

Problem Set 5 Solutions
Heteronuclear Correlation Spectroscopy

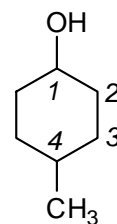
1. a. We can identify a number of peaks that belong to solvents and byproducts:

proton	δ (ppm)
THF	3.60
THF	1.74
cyclohexane	1.44
butane	1.28
butane	0.89
TMS	0
H _[3]	7.27
H _[4]	7.09
H _[5]	7.49

carbon	δ (ppm)
THF	68.1
THF	27.6
cyclohexane	26.2
butane	25.5
butane	14.0
TMS	0
C _[2]	175.2
C _[3]	136.1
C _[4]	126.8
C _[5]	129.3

- b. 2-Thiophenyllithium was formed. It's the only one that has a continuous set of coupled protons in the backbone.
- c. See table above.
- d. Although the HMBC method is designed to discriminate against 1J coupling, it sometimes breaks through the J filter. When it does, the crosspeaks look like pairs of peaks centered at the crosspeak position.

2. a. There are very few resonances in the NMRs, and that means the molecule has to be symmetric; the only possibility is 4-methyl-cyclohexanol.



4-methyl-cyclohexanol

proton	δ (ppm)
H _[1]	3.50
H _[2a]	1.91
H _[2b]	1.23
H _[3a]	1.67
H _[3b]	0.94
H _[4]	1.28
-CH ₃	0.85

carbon	δ (ppm)
C _[1]	71.0
C _[2]	35.7
C _[3]	33.5
C _[4]	31.9
-CH ₃	22.1

- b. I don't think you can tell, because of the difficulty of determining $J(H_3, H_4)$.