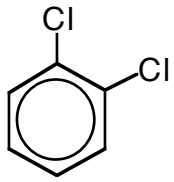
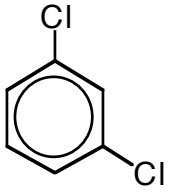
Problem 76, Chemistry 301X-2006

You are given three bottles containing *o*-dichlorobenzene (**1**), *m*-dichlorobenzene, (**2**), and *p*-difluorobenzene (**3**), along with broad-band decoupled ^{13}C NMR spectra of the three isomers. Use symmetry to assign the three spectra (**A**, **B**, **C**) to the three compounds and explain your reasoning.

A: δ = 127.0, 128.9, 130.6, 135.1 ppm; **B**: δ = 127.7, 130.5, 132.6 ppm; **C:** δ **=** 116.5, 159.1 ppm.



1

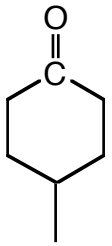


2

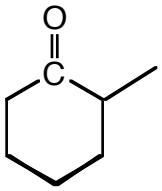
3

Would this same technique (looking at symmetry) allow you to assign the spectra of 4-methylcyclohexanone, 2-methylcyclohexanone, and 2,3-dimethylcyclopentanone, **A**, **B**, and **C**? If not, suggest an experiment, involving only ^{13}C NMR spectroscopy, that would let you finish the job.

A



B



C