

## 2.9: Illustrative Analysis of a Reaction Product

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Nuclear magnetic resonance spectra are often useful for characterization of complex reaction mixtures. For example, in an exploratory methylation of phenyldimethylcarbinol, distillation of the reaction products gave two principal fractions with NMR spectra as shown in Fig. 2-12. These spectra can be quite well analyzed even without the aid of separate spectra of the pure component.<sup>22</sup> The presence of resonance lines in the vinyl hydrogen region indicates the formation of some  $\alpha$ -methylstyrene, while the band at +100 cps shows the presence of O-CH<sub>3</sub>. The methyl absorptions of the ether are separated somewhat from those of the alcohol, and we can assign the higher of the two peaks in the first fraction to the ether, since it is roughly twice the O-CH<sub>3</sub> resonance. Each fraction shows O-H lines which are shifted somewhat from one fraction to the other by chemical shift changes associated with solvent changes as explained earlier for ethanol. From the NMR spectra, we can conclude that the first and second fractions have approximately the compositions 53 and 23 percent methyl phenyldimethylcarbinyl ether, 35 and 77 percent phenyldimethylcarbinol, and 12 and 0 per cent  $\alpha$ -methylstyrene, respectively.

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22 Unpublished experiments by M. C. Caserio.

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