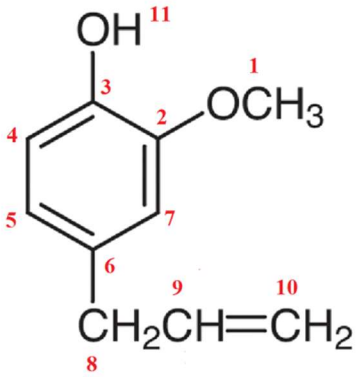
Eugenol



	^{1}H chemical shift	^{13}C chemical shift
1	3.764 (singlet)	55.598
2, 3	n/a	146.411 or 143.798
4, 5, 7	6.600-6.889	111.082, 114.258, 121.030
6	n/a	131.701
8	3.276 (doublet)	39.642
9	5.179-5.985	137.730
10	4.946-5.147	115.262

Notes:

Note that the carbon spectrum shows ten signals within the aromatic and alkene regions. Clearly, six of these arise from the benzene ring and two arise from the alkene carbon atoms. The HETCOR spectrum allows these to be sorted out.

Within the benzene ring, three carbon atoms do not have attached hydrogen atoms (C2, C4 and C6) and can readily be identified using the HETCOR spectrum, since no correlations should be observed. These occur at 131.701, 143.798, and 146.411 ppm. The latter two can be assigned to C2 and C3, but additional data would be needed to make specific assignments. The one at 146.411 is assigned to C6 since it shifted furthest upfield.

Within the benzene ring, three carbon atoms do have attached hydrogen atoms (C4, C5, and C7) and should show correlations to the aromatic region of the proton spectrum. These occur at 111.082, 114.258, and 121.030 ppm and show correlations to the proton spectrum at 6.600-6.889 ppm. Unfortunately, specific assignments cannot be made without additional data.

The proton spectrum shows two multiplets in the alkene region at 4.946-5.147 ppm and 5.179-5.985 ppm. The corresponding carbon atoms are readily identified using the HETCOR spectrum; these occur at 137.730 ppm (C9) and 115.626 ppm (C10). Note that the two C10 protons are nonequivalent (one trans to the CH and one cis to the CH). These are indistinguishable here but might be resolved on a higher-field nmr.

The singlet in the proton spectrum at 3.764 ppm is readily assigned to H1; this shows a correlation to the carbon at 55.598 ppm.

The doublet at 3.276 is assigned to the H8 (since it is split only by the single H9 hydrogen.) This shows a correlation to the carbon at 39.642 ppm.