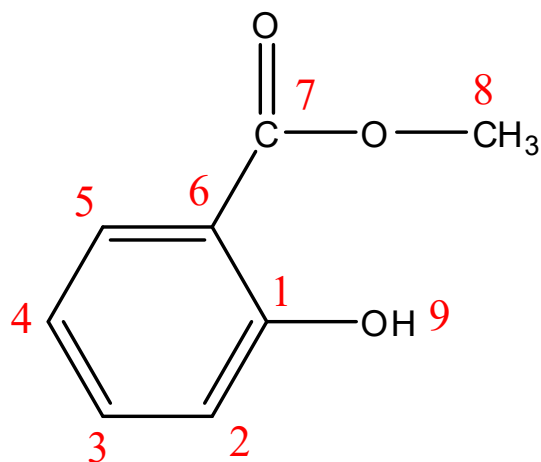


Methyl Salicylate



Atom	¹ H Chemical Shift	¹³ C Chemical Shift
1	n/a	161.463
2	6.722 – 6.990 (overlapped)	117.312
3	7.303 – 7.496	135.418
4	6.722 – 6.990 (overlapped)	118.880
5	7.721 – 7.829 (doublet of doublets)	129.691
6	n/a	112.168
7	n/a	170.345
8	3.872 (singlet)	51.920
9	10.756 (singlet)	n/a

Three ¹³C signals do not show correlations in the HETCOR spectrum – 112.168, 161.463, and 170.345 ppm. The one shifted furthest downfield (170.345) is assigned to C7 (the carbonyl). The one shifted furthest upfield (112.168) is assigned to C6 since it is not attached to an electronegative element. This leaves the one at 161.463 to be assigned to C1.

Protons 2 and 5 are split by one large (ortho) and one smaller (meta) coupling and should appear as a doublet of doublets

Protons 3 and 4 are split by two large (ortho) and one smaller (meta) couplings and will exhibit more complex splitting.

Electronegative groups (such as the –OH group) cause protons in the *meta* position to be shifted further downfield, so the doublet of doublets at 7.721-7.829 ppm (the furthest downfield protons) is assigned to the C5 proton.

The signals at 7.721 – 7.829 (the next furthest downfield protons) must arise from H3 or H4; these are assigned to H3 since it also *meta* to the –OH group.

The ^1H signals at 6.722 – 6.990 show correlations to two ^{13}C signals at 117.312 and 118.880 ppm and must be overlapped. These could not be resolved.

A long-range proton-carbon (COLOC) showed a correlation between the H9 and the carbon resonance at 117.312 ppm, allowing this to be assigned to C2.