

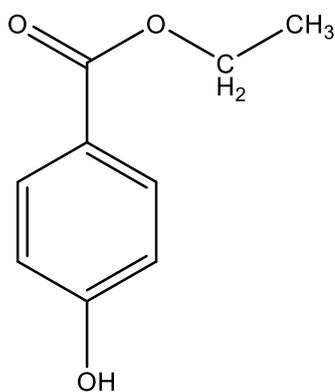
Answer on Question #81464 – Chemistry – Organic Chemistry

Task:

Provide a structure for the following compound: $C_9H_{10}O_3$; IR: 2400–3200, 1700, 1630 cm^{-1} ; 1H NMR: δ 1.53 (3H, t, $J = 8$ Hz); δ 4.32 (2H, q, $J = 8$ Hz); δ 7.08, δ 8.13 (4H, pair of leaning doublets, $J = 10$ Hz); δ 10 (1H, broad, disappears with D_2O shake).

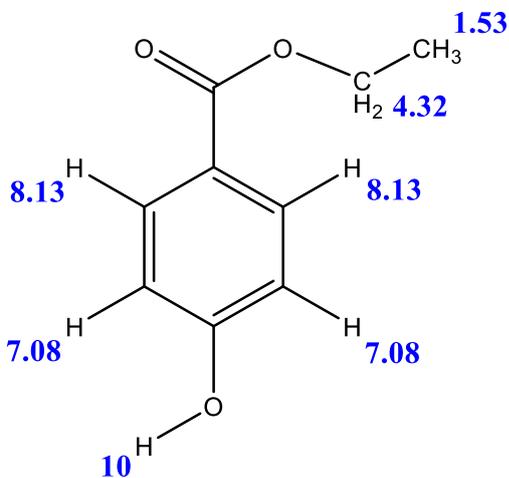
Solution:

Structure for the compound, $C_9H_{10}O_3$:



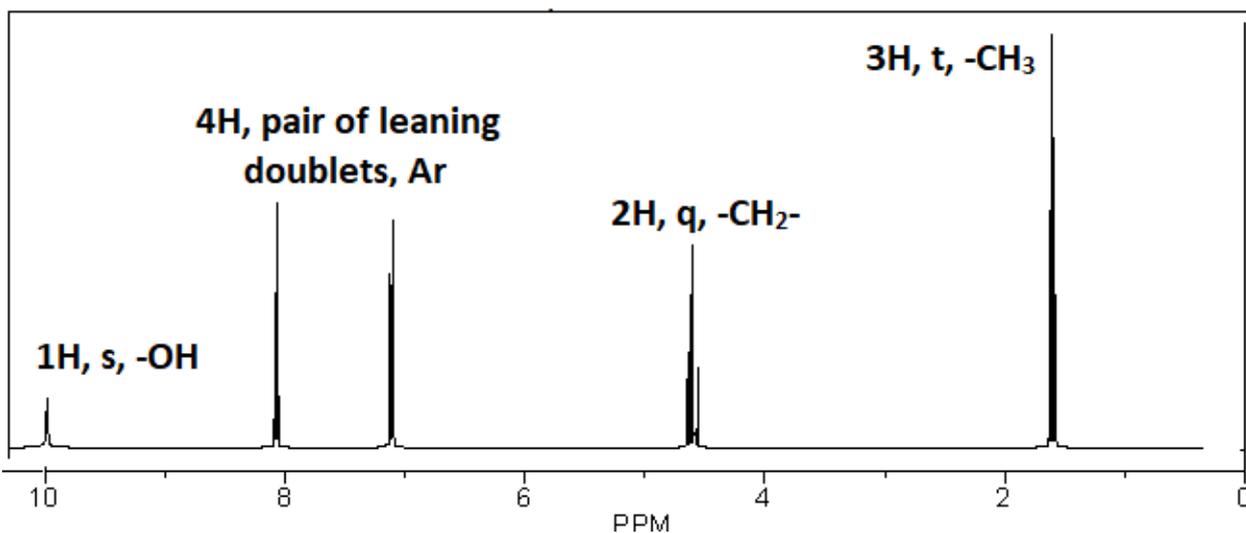
ethyl 4-hydroxybenzoate

1H NMR: δ 1.53 (3H, t, $J = 8$ Hz); δ 4.32 (2H, q, $J = 8$ Hz); δ 7.08, δ 8.13 (4H, pair of leaning doublets, $J = 10$ Hz); δ 10 (1H, broad, disappears with D_2O shake).



If a drop of D₂O is added to the NMR sample tube and the tube is shaken, the OH protons rapidly exchange with the protons of D₂O to form OD groups on the alcohol. As a result, the OH resonance disappears when the spectrum is rerun.

Schematic ¹H NMR spectrum of C₉H₁₀O₃:



IR: 2400–3200, 1700, 1630 cm⁻¹

1700 cm⁻¹ : C=O stretch

1630 cm⁻¹ : C=C stretch

2400–3200 cm⁻¹ : =C-H stretch

The =C–H stretch in aromatics is observed at 3100-3000 cm⁻¹

Aromatic hydrocarbons show absorptions in the regions 1700-1585 cm⁻¹ and

1500-1400 cm⁻¹ due to carbon-carbon stretching vibrations in the aromatic ring

For aromatics:

- C–H stretch from 3100-3000 cm⁻¹
- overtones, weak, from 2000-1665 cm⁻¹
- C–C stretch (in-ring) from 1600-1585 cm⁻¹
- C–C stretch (in-ring) from 1500-1400 cm⁻¹
- C–H "oop" from 900-675 cm⁻¹