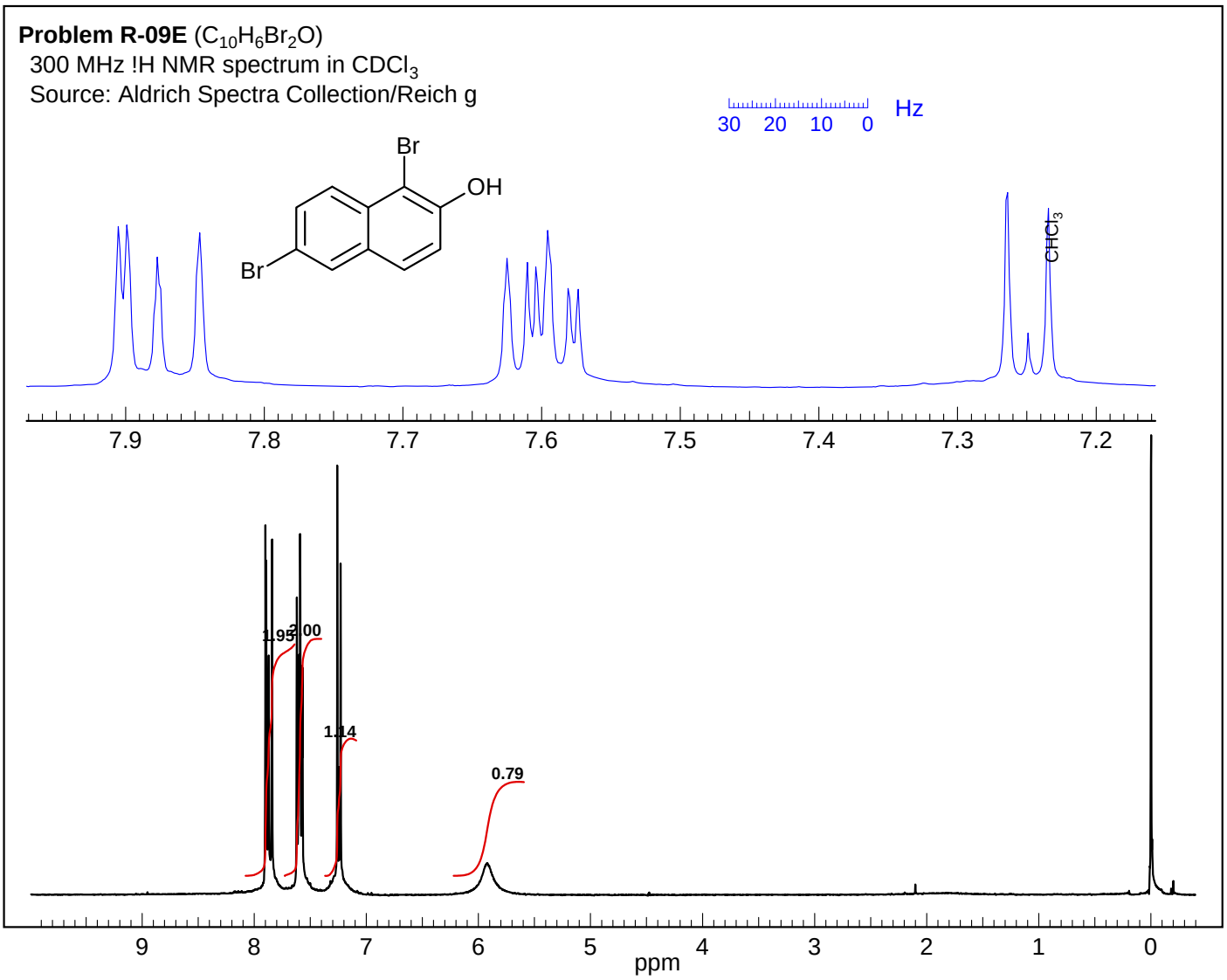
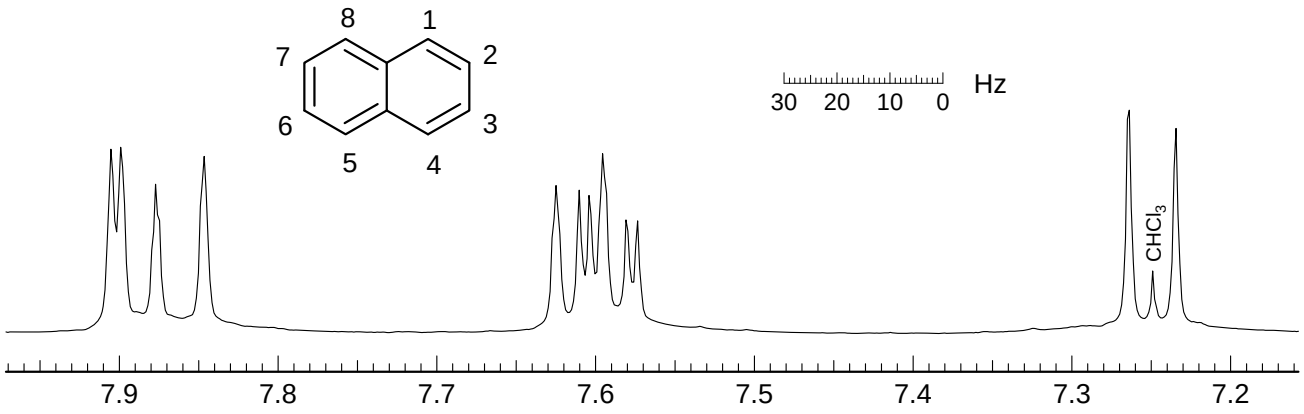


PLT ex-1-2009-10-gq.plt

Problem R-09E ($C_{10}H_6Br_2O$). Shown below is the aromatic region of the 300 MHz ^1H NMR spectrum of a trisubstituted naphthalene (the substituents are **Br**, **Br** and **OH**). Your task is to analyze the NMR spectrum, and determine the substitution pattern (Source: Aldrich Spectral Viewer).



(a) For each of the 8 positions on the naphthalene as defined above, place either an X if there is a substituent, or the NMR signal (δ , multiplicity and *J* values). If there is more than one plausible structure asignment, draw the alternative structure, and indicate your preference. To simplify grading, please put the substituents on the lowest numbered positions (e.g., on carbon 1 rather than on 4).

1 _____

2 _____

3 _____

4 _____

5 _____

6 _____

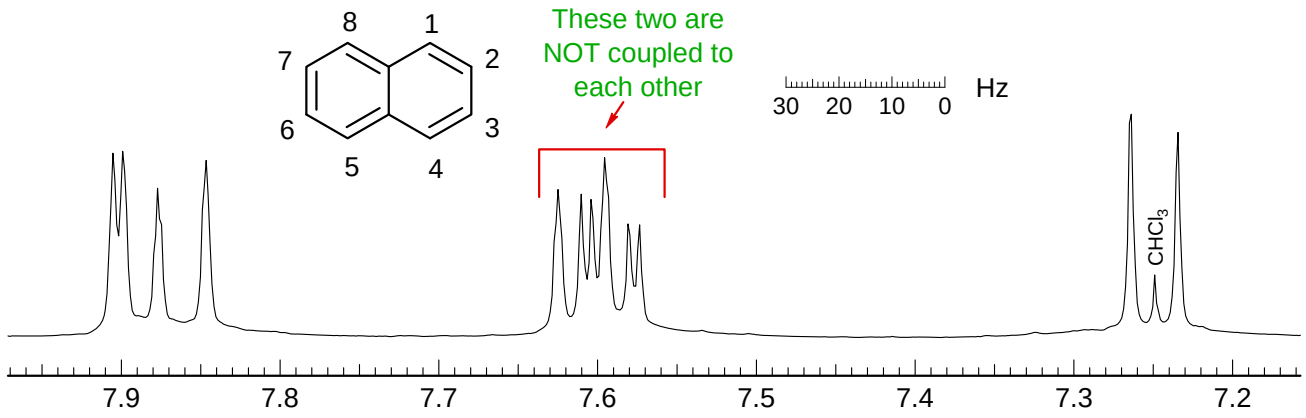
7 _____

8 _____

(b) From a qualitative consideration of chemical shift effects (please don't attempt to do chemical shift calculations on all possible isomers) suggest which of the three occupied positions is most likely to be the OH, and give your reasoning.

17

Problem R-09E ($C_{10}H_6Br_2O$). Shown below is the aromatic region of the 300 MHz ^1H NMR spectrum of a trisubstituted naphthalene (the substituents are **Br**, **Br** and **OH**). Your task is to analyze the NMR spectrum, and determine the substitution pattern (Source: Aldrich Spectral Viewer).



(a) For each of the 8 positions on the naphthalene as defined above, place either an X if there is a substituent, or the NMR signal (δ , multiplicity and *J* values). If there is more than one plausible structure asignment, draw the alternative structure, and indicate your preference. To simplify grading, please put the substituents on the lowest numbered positions (e.g., on carbon 1 rather than on 4).

1	X (Br)	X (Br)
2	X (OH)	X (OH)
3	δ 7.25,d, J = 9 Hz	δ 7.25,d, J = 9 Hz
4	δ 7.61, d, J = 9 Hz	δ 7.61,d (m?), J = 9 Hz
5	δ 7.90, d, J = 2 Hz	δ 7.86, d, J = 9 Hz
6	X (Br)	δ 7.59,dd, J = 9, 2 Hz
7	δ 7.59,dd, J = 9, 2 Hz	X (Br)
8	δ 7.86, d, J = 9 Hz	δ 7.90, d, J = 2 Hz

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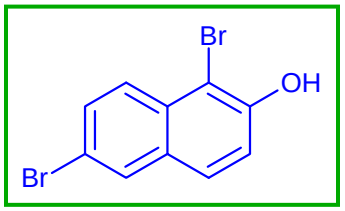
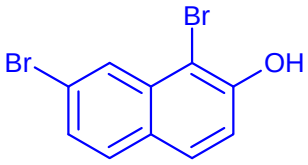
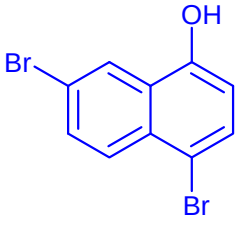
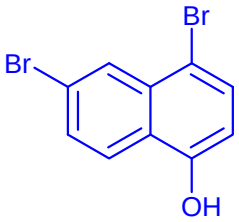




Both OK, Br-OH swapped also works

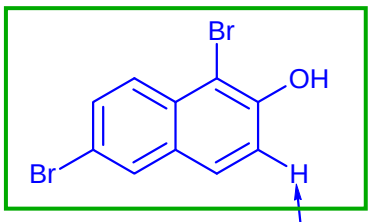




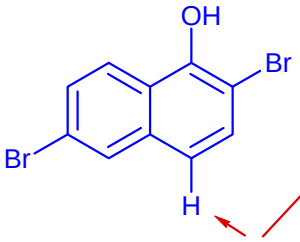
Reasonable, but J_{HH} would be smaller (6 Hz instead of 9 Hz, as observed)

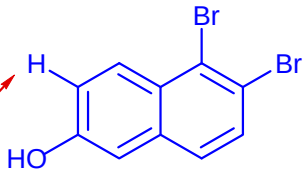
(b) From a qualitative consideration of chemical shift effects (please don't attempt to do chemical shift calculations on all possible isomers) suggest which of the three occupied positions is most likely to be the OH, and give your reasoning.

4



Should be most upfield proton (as observed)





Should be most upfield proton