Homework 4 Key

Solve the following structures from their spectra. Correlate the NMR peaks with the structure. Make a summary table for each (both 1-H and C-13) and give a proper name for each compound.

Molecular Formula	Proton chemical shifts (multiplicity, integration) multiplicity d-doublet t-triplet q-quartet m-multiplet	Carbon chemical shifts (DEPT results, intensity) u-up, n-no peak, d-down three results from bottom to top on DEPT spectra
a) C_4H_9Br	1.0 (t, 3), 1.7 (d, 3), 1.8 (m, 2), 4.1 (m, 1)	12 (unu, 1), 26 (unu, 1), 34 (und, 1), 53 (uuu, 1)
b) $C_4H_8Br_2$	2.0 (t, 4), 3.4 (t, 4)	31.0 (und, 2), 32.5 (und, 2)
c) C_3H_7Br	1.3 (d, 6), 3.8 (m, 1)	28.5 (uuu, 1), 45.4 (unu, 2)
d) $C_5H_{11}Cl$	0.9 (d, 6), 1.4 (m, 1), 1.9 (q, 2), 3.6 (t, 2)	22 (unu, 2), 26 (uuu, 1), 42 (und, 1), 43 (und, 1)

a) 2-bromobutane: $CH_3CH_2CHBrCH_3$

A B C D

δ (ppm)	# peaks	# neigh H	Integr	H label
1.0	3	2	3	A
1.7	2	1	3	D
1.8	multi	4	2	B
4.1	multi	5	1	C

δ (ppm)	C label
12	A
26	D
34	B
53	C

b) 1,4-dibromobutane: $CH_2BrCH_2CH_2CH_2Br$

A B B A

δ (ppm)	# peaks	# neigh H	Integr	H label
2.0	3	2	2	B
3.4	3	2	2	A

δ (ppm)	C label
31	B
32.5	A

c) 2-bromopropane: $CH_3CHBrCH_3$

A B A

δ (ppm)	# peaks	# neigh H	Integr	H label
1.3	2	1	6	A
3.8	7	6	1	B

δ (ppm)	C label
28.5	A
45.4	B

d) 1-chloro-3-methylbutane: $(CH_3)_2CHCH_2CH_2Cl$

A B C D

δ (ppm)	# peaks	# neigh H	Integr	H label
0.9	2	1	6	A
1.4	multi	8	1	B
1.9	4	3	2	C
3.6	7	2	2	D

δ (ppm)	C label
22	A
26	B
42	C
43	D