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Chapter One, Problem B

Worksheet, step one: In this case, the IHD = 1. Only13 of the H's are attached to carbon, so one must be attached to the O – this must be an alcohol.

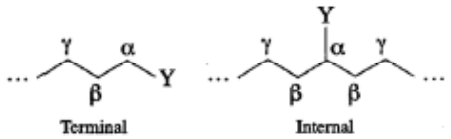
$C_6H_{14}O$

11, q (2)
23, t (2)
44, d
65, t

Worksheet, step two: The IHD = 0.

Worksheet, step three: Using the same approach as for problem A, we can calculate

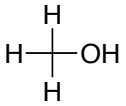
Table C.11 Incremental Substituent Effects (ppm) on Replacement of H by Y in Alkanes



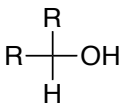
	α		β		γ
Y	TERMINAL	INTERNAL	TERMINAL	INTERNAL	
CH_3	+ 9	+ 9	+ 6	+ 6	−2
$CH=CH_2$	+20		+ 6		−0.5
C CH	+ 4.5		+ 5.5		−3.5
COOH	+21	+16	+3	+ 2	−2
COO^-	+25	+20	+5	+ 3	−2
COOR	+20	+17	+3	+ 2	−2
COCl	+33	28		+ 2	
$CONH_2$	+22		+ 2.5		−0.5
COR	+30	+24	+ 1	+ 1	−2
CHO	+31		0		−2
Phenyl	+23	+17	+ 9	+ 7	−2
OH	+48	+41	+10	+ 8	−5
OR	+58	+51	+ 8	+ 5	−4
OCOR	+51	+45	+ 6	+ 5	−3
NH_2	+29	+24	+11	+10	−5
NH_3	+26	+24	+ 8	+ 6	−5
NHR	+37	+31	+ 8	+ 6	−4
NR_2	+42		+ 6		−3
NR_3	+31		+ 5		−7
NO_2	+63	+57	+ 4	+ 4	
CN	+ 4	+ 1	+ 3	+ 3	−3
SH	+11	+11	+12	+11	−4
SR	+20		+ 7		−3
F	+68	+63	+ 9	+ 6	−4
Cl	+31	+32	+11	+10	−4
Br	+20	+25	+11	+10	−3
I	− 6	+ 4	+11	+12	−1

generic chemical shift for alcohol. Using Table C11, note that the first letter in the functional group, on the left hand side of the column, is the atom directly attached to carbon. The α-shift for OH is + 48, so table of generic chemical shifts for OH looks like this.

Generic Chemical Shifts: Alcohol

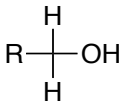


46, q

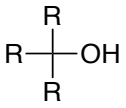


71, d

Inspecting the data, the signal that matches, in chemical shift and multiplicity, is 65, t. So, we know that we have $–CH_2-OH$.

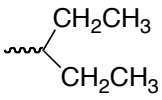


62, t

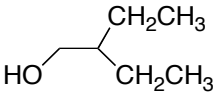


80, s

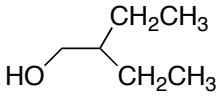
Worksheet, Step 4a: There is a pair of symmetrical methyl groups, at 11, q (2). There is also a pair of symmetrical methylenes, at 23, t (2). It follows that there are symmetrical ethyl groups in this molecule. There is no other symmetry, so they must be attached to the same carbon.

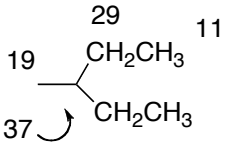


Worksheet, Step 5: There is only one way to assemble the molecule.

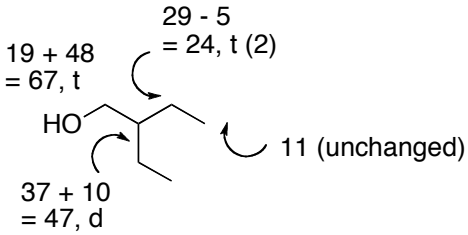


Again, it is instructive to calculate "precise" ^{13}C chemical shifts, and compare the tabulated data to that for the unknown. In this case, the starting hydrocarbon is 3-methylpentane (following page).





We add the appropriate and α, β, and γ shifts from Table C11 to the data from Table C10 to calculate the more precise ^{13}C chemical shifts, and then put the results in table form.



Calculated	Actual
11, q (2)	11, q (2)
24, t (2)	23, t (2)
47, d	44, d
67, t	65, t

Table C.10 The ^{13}C Shifts for Some Linear and Branched-Chain Alkanes (ppm from TMS)

COMPOUND	C-1	C-2	C-3	C-4	C-5
Methane	−2.3				
Ethane	5.7				
Propane	15.8	16.3	15.8		
Butane	13.4	25.2	25.2		
Pentane	13.9	22.8	34.7	22.8	13.9
Hexane	14.1	23.1	32.2	32.2	23.1
Heptane	14.1	23.2	32.6	29.7	32.6
Octane	14.2	23.2	32.6	29.9	29.9
Nonane	14.2	23.3	32.6	30.0	30.3
Decane	14.2	23.2	32.6	31.1	30.5
Isobutane	24.5	25.4			
Isopentane	22.2	31.1	32.0	11.7	
Isohexane	22.7	28.0	42.0	20.9	14.3
Neopentane	31.7	28.1			
2,2-Dimethylbutane	29.1	30.6	36.9	8.9	
3-Methylpentane	11.5	29.5	36.9	(18.8, 3-CH_3)	
2,3-Dimethylbutane	19.5	34.3			
2,2,3-Trimethylbutane	27.4	33.1	38.3	16.1	
2,3-Dimethylpentane	7.0	25.3	36.3	(14.6, 3-CH_3)	

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