

Table 1. The BS Method for sp^3 Carbon Atoms

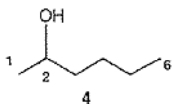
A, A', B, B', C are atoms other than H.

base = 0 ppm

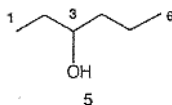
base structure: $^{13}\text{C}[-\text{A}-\text{B}-\text{C}]_4$

A = B = 7.5 ppm

sp^3 Corrections	[Code]
1. C-Me group not attached to a $-\text{CH}_2-$: -2.4 ppm.	[C-MeNA]
2. C-Me group attached to a $-\text{CH}_2-$: -0.4 ppm	[C-MeAT]
3. C(13) is a CH_3 group with a C carbon atom: -0.4 ppm	[Me]
4. C(13) is a $-\text{CH}_2-$ and the third atom other than H in the chain: 2.5 ppm.	[3rdM]
5. C(13) is tertiary: -1.5 ppm \times # of B atoms	[T]
6. C(13) is quaternary: -4.4 ppm \times # of B atoms	[Q]
7. C(13) is allylic or <i>trans</i> -allylic: 5 ppm	[AL]
8. C(13) is <i>cis</i> -allylic: -1.25 ppm	[c-AL]
9. C(13) is propargylic: -10 ppm	[P]
10. C(13) is in a cyclopropane ring: -32.6 ppm	[R3]
11. C(13) is in a cyclobutane ring: -6.7 ppm	[R4]
12. C(13) is in a cyclopentane ring: -3.5 ppm	[R5]
13. C(13) is in a cyclohexane ring: -2.2 ppm	[R6]
14. C(13) is in a cycloheptane ring: -0.6 ppm	[R7]
15. C(13) is on all axis of symmetry: -2.7 ppm	[S]
16. A- sp^3 oxygen atoms: 37.5 ppm \times # of oxygen atoms	[AO]
17. A- sp^3 nitrogen atoms: 22.5 ppm \times # of nitrogen atoms	[AN]
18. A- sp^3 bromine atoms: 22.5 ppm \times # of bromine atoms	[ABr]
19. A- sp^3 chlorine atoms: 30 ppm \times # of chlorine atoms	[ACl]
20. B- sp^2 oxygen atoms of an aldehyde or ketone: 6.1 ppm	[BO]
21. C- sp^3 oxygen atoms: -3.2 ppm \times # of oxygen atoms	[CO]
22. C- sp^2 oxygen atoms: -5.0 ppm \times # of oxygen atoms	[Csp ² O]



Carbon	BS Method	calc'd ppm	(exp) ppm
1	1A + 2B + Me	21.1	(23.3)
2	3A + 1B + T + AO	66.0	(67.2)
3	2A + 3B + (C-MeAT) + 3rdM	39.6	(39.2)
4	2A + 2B + (C-MeNA) + 3rdM + CO	26.8	(28.3)
5	2A + 1B	22.5	(22.9)
6	1A + 1B + Me	14.6	(13.9)



Carbon	BS Method	calc'd ppm	(exp) ppm
1	1A + 1B + Me + CO	11.4	(9.9)
2	2A + 2B	30	(30.3)
3	3A + 2B + (C-MeAt) + T + AO	71.6	(72.3)
4	2A + 3B + (C-MeAT) + 3rdM	39.6	(39.4)
5	2A + 1B + CO	19.3	(19.4)
6	1A + 1B + Me	14.6	(14.0)