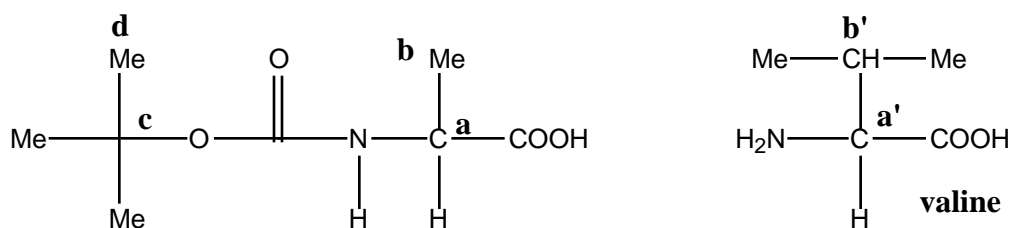


Example 2: The estimation of the C-NMR chemical shifts for the carbons (a) and (b) in the N-t-butoxycarbonylalanine using the shifts of valine as the base.



The a' and b' C-atoms in valine resonate at 61.6 and 30.2 ppm, respectively.

Carbon (a)

base value	61.6	
-COOH (in base)		
-Me (in base)		
-N< (in base)		
-COO	2.0	
no group (COO is and)		
-Calkyl	0.3	
S(CH, N has 2 Cs)	-3.7	
- 2 -C (in valine nut not in...)	-18.8	NEW!
- S(CH, 3)	+8.5	NEW!
Estimated:	49.9	
Experimental:	49.0	

Exercise this method for carbon (b) using the base value 30.2 ppm.