

^{13}C -NMR ABSORPTIONS OF MAJOR FUNCTIONAL GROUPS

The table below lists the range of ^{13}C chemical shifts δ in parts per million relative to tetramethylsilane, in descending order, for various functional groups. Examples of simple compounds for each family are given to illustrate the correlations. The shifts for the carbons of interest, which are italicized, are given in parentheses; when two or more values appear, they refer to the sequence of italicized carbon atoms from left to right in the formula.

δ (ppm)	Group	Family	Example (δ of italicized carbon)				
220-165	$>\text{C}=\text{O}$	Ketones	$(\text{CH}_3)_2\text{CO}$	(206.0)			
			$(\text{CH}_3)_2\text{CHCOCH}_3$	(212.1)			
			CH_3CHO	(199.7)			
		Aldehydes	α,β -Unsaturated carbonyls	$\text{CH}_3\text{CH}=\text{CHCHO}$	(192.4)		
				$\text{CH}_2=\text{CHCOCH}_3$	(169.9)		
		Carboxylic acids	Amides	HCO_2H	(166.0)		
				$\text{CH}_3\text{CO}_2\text{H}$	(178.1)		
		140-120	$>\text{C}=\text{C}<$	Alkenes	HCONH_2	(165.0)	
					CH_3CONH_2	(172.7)	
				Aromatic	Esters	$\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_3$	(170.3)
					$\text{CH}_2=\text{CHCO}_2\text{CH}_3$	(165.5)	
					C_6H_6	(128.5)	
		125-115 80-70 70-45 40-20 30-15 30-(-2.3)	$-\text{CN}$ $-\text{CC}-$ $-\text{C}-\text{O}$ $-\text{C}-\text{NH}_2$ $-\text{S}-\text{CH}_3$ $-\text{C}-\text{H}$	Alkenes	$\text{CH}_2=\text{CH}_2$	(123.2)	
$\text{CH}_2=\text{CHCH}_3$	(115.9, 136.2)						
Nitriles	Alkynes			$\text{CH}_2=\text{CHCH}_2\text{Cl}$	(117.5, 133.7)		
				$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$	(132.7)		
Esters	Alkynes			CH_3-CN	(117.7)		
				HCCH	(71.9)		
Alcohols	Amines			CH_3CCH_3	(73.9)		
				$\text{CH}_3\text{OOCH}_2\text{CH}_3$	(57.6, 67.9)		
Alcohols	Amines			HOCH_3	(49.0)		
				HOCH_2CH_3	(57.0)		
Sulfides (thioethers)	Alkanes, cycloalkanes	CH_3NH_2	(26.9)				
		$\text{CH}_3\text{CH}_2\text{NH}_2$	(35.9)				
Alkanes, cycloalkanes	Alkanes, cycloalkanes	$\text{C}_6\text{H}_5-\text{S}-\text{CH}_3$	15.6				
		CH_4	(-2.3)				
Cyclohexane	Cyclohexane	CH_3CH_3	(5.7)				
		$\text{CH}_3\text{CH}_2\text{CH}_3$	(15.8, 16.3)				
		$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	(13.4, 25.2)				
		$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	(13.9, 22.8, 34.7)				
		Cyclohexane		(26.9)			

References

1. Yoder, C. H. and Schaeffer, C. D., Jr., *Introduction to Multinuclear NMR: Theory and Application*, Benjamin/Cummings, Menlo Park, CA, 1987.
2. Silverstein, R. M., Bassler, G. C., and Morrill, T. C., *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, New York, 1981.
3. Brown, D. W., A Short Set of ^{13}C NMR Correlation Tables, *J. Chem. Educ.*, 62, 209, 1985.