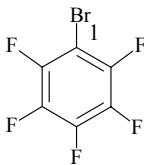
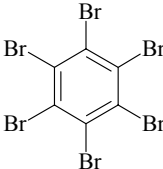
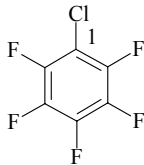
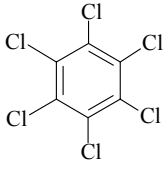
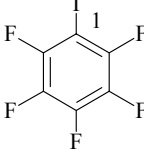
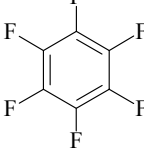
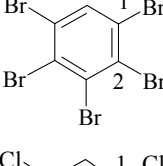
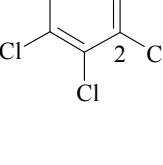
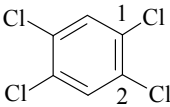
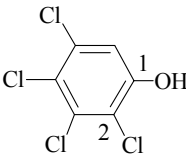
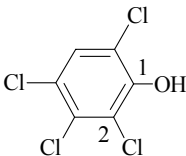
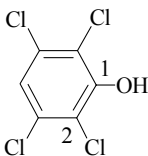
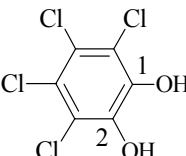
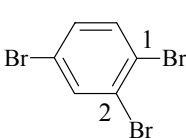
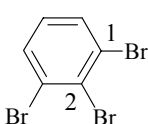
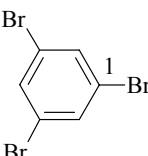
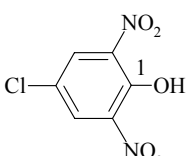
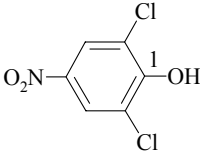
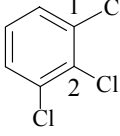
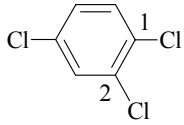
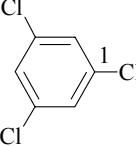
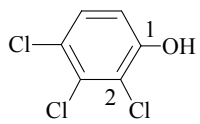
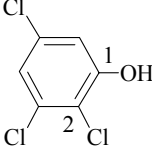
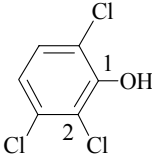
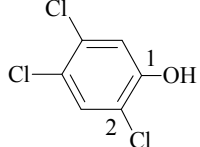
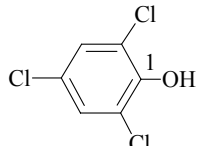


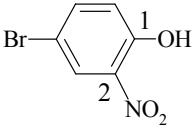
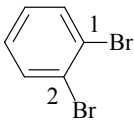
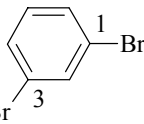
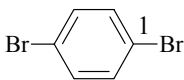
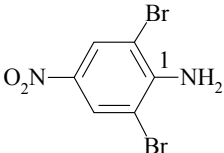
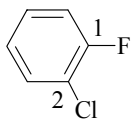
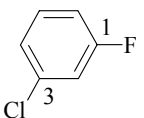
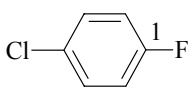
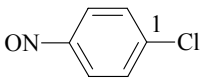
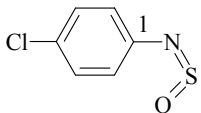
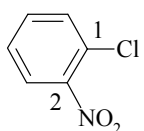
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
C_6BrF_5		Neat	94.7(C1) 145.6(C2/6) 138.4(C3/5) 141.3(C4)	73Bri
C_6Br_6		CDCl_3	128.5(C1-6)	85Tak
C_6ClF_5		Neat	108.0(C1) 144.8(C2/6) 138.3(C3/5) 140.7(C4)	73Bri
C_6Cl_6		CDCl_3	132.3(C1-6)	85Tak
$\text{C}_6\text{F}_5\text{I}$		Neat	65.7(C1) 147.9(C2/6) 137.7(C3/5) 142.4(C4)	73Bri
C_6F_6		Neat	138.3(C1-6)	73Bri
C_6HBr_5		CDCl_3	124.7(C1/5) 127.8(C2/4) 129.9(C3) 135.5(C6)	85Tak
C_6HCl_5		CDCl_3	132.2(C1/5) 131.6(C2/4) 134.4(C3) 128.8(C6)	85Tak

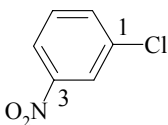
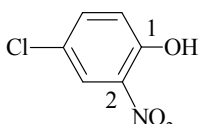
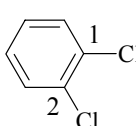
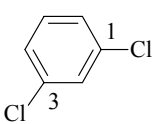
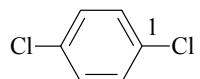
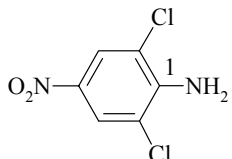
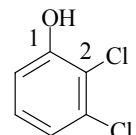
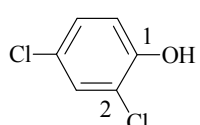
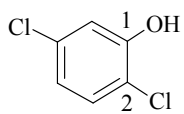
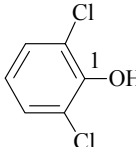
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{HCl}_5\text{O}$		CDCl_3	148.3(C1) 119.9(C2/6) 131.6(C3/5) 125.2(C4)	80Ilc
$\text{C}_6\text{H}_2\text{BrCl}_2\text{NO}_2$		CDCl_3	131.2(C1) 137.5(C2/6) 122.9(C3/5) 146.6(C4)	89Str
$\text{C}_6\text{H}_2\text{BrI}_2\text{NO}_2$		CDCl_3	144.1(C1) 99.4(C2/6) 134.3(C3/5) 146.2(C4)	89Str
$\text{C}_6\text{H}_2\text{Br}_3\text{NO}_2$		CDCl_3	135.6(C1) 126.7(C2/6) 126.8(C3/5) 146.6(C4)	89Str
$\text{C}_6\text{H}_2\text{Br}_4$		CDCl_3	124.7(C1/4) 129.0(C2/3) 132.7(C5/6)	85Tak
$\text{C}_6\text{H}_2\text{Br}_4$		CDCl_3	126.5(C1/3) 126.7(C2) 134.8(C4/6) 121.3(C5)	85Tak
$\text{C}_6\text{H}_2\text{Br}_4$		CDCl_3	124.3(C1/2/4/5) 137.1(C3/6)	85Tak
$\text{C}_6\text{H}_2\text{Cl}_4$		CDCl_3	132.5(C1/4) 133.1(C2/3) 128.3(C5/6)	85Tak
$\text{C}_6\text{H}_2\text{Cl}_4$		CDCl_3	134.7(C1/3) 130.3(C2) 128.6(C4/6) 132.7(C5)	85Tak

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_2\text{Cl}_4$		CDCl_3	131.6(C1/2/4/5) 132.2(C3/6)	85Tak
$\text{C}_6\text{H}_2\text{Cl}_4\text{O}$		Ac-d_6	153.4(C1) 120.5(C2) 133.0(C3) 122.5(C4) 131.8(C5) 116.4(C6)	80Knu
$\text{C}_6\text{H}_2\text{Cl}_4\text{O}$		Ac-d_6	149.7(C1) 122.5(C2) 130.3(C3) 123.9(C4) 128.8(C5) 121.0(C6)	80Knu
$\text{C}_6\text{H}_2\text{Cl}_4\text{O}$		Ac-d_6	151.8(C1) 120.0(C2/6) 131.6(C3/5) 121.8(C4)	80Knu
$\text{C}_6\text{H}_2\text{Cl}_4\text{O}_2$		Ac-d_6	143.0(C1/2) 119.5(C3/6) 122.5(C4/5)	80Knu
$\text{C}_6\text{H}_3\text{Br}_3$		CDCl_3	123.6(C1) 125.7(C2) 136.0(C3) 121.2(C4) 131.6(C5) 134.5(C6)	85Tak
$\text{C}_6\text{H}_3\text{Br}_3$		CDCl_3	126.1(C1/3) 127.5(C2) 132.4(C4/6) 129.0(C5)	85Tak
$\text{C}_6\text{H}_3\text{Br}_3$		CDCl_3	123.2(C1/3/5) 132.9(C2/4/6)	72Jon
$\text{C}_6\text{H}_3\text{ClN}_2\text{O}_5$		CDCl_3	148.2(C1) 138.0(C2/6) 131.5(C3/5) 124.6(C4)	80Ilc

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_3\text{Cl}_2\text{NO}_3$		CDCl_3	153.7(C1) 121.8(C2/6) 124.4(C3/5) 140.9(C4)	80Ilc
$\text{C}_6\text{H}_3\text{Cl}_3$		CDCl_3	134.3(C1/3) 131.6(C2) 128.6(C4/6) 127.5(C5)	72Jon
$\text{C}_6\text{H}_3\text{Cl}_3$		CDCl_3	131.0(C1) 133.7(C2) 130.1(C3) 132.9(C4) 127.8(C5) 130.9(C6)	85Tak
$\text{C}_6\text{H}_3\text{Cl}_3$		CDCl_3	135.6(C1/3/5) 127.2(C2/4/6) $^1J(\text{C2}, \text{H2})=172.5$ $^3J(\text{C2}, \text{H4})=5.3$	77Ner
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		Ac-d_6	153.6(C1) 121.1(C2) 131.4(C3) 123.6(C4) 128.8(C5) 115.8(C6)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		Ac-d_6	155.3(C1) 118.8(C2) 133.8(C3) 121.0(C4) 132.7(C5) 115.4(C6)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		Ac-d_6	150.8(C1) 121.2(C2) 131.8(C3) 121.7(C4) 128.6(C5) 120.6(C6)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		Ac-d_6	153.0(C1) 120.4(C2) 131.0(C3) 122.7(C4) 131.0(C5) 118.2(C6)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		CDCl_3	147.1(C1) 121.8(C2/6) 128.2(C3/5) 125.5(C4)	80Ilc

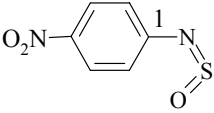
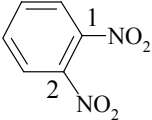
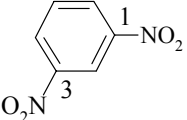
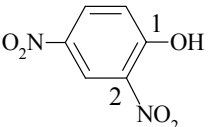
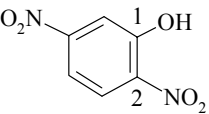
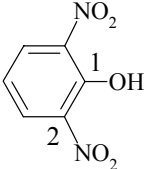
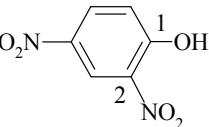
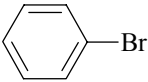

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}$		Ac-d_6	156.9(C1) 116.8(C2/6) 134.0(C3/5) 121.1(C4)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}_2$		Ac-d_6	145.5(C1) 143.0(C2) 120.6(C3) 121.2(C4) 122.7(C5) 115.0(C6)	80Knu
$\text{C}_6\text{H}_3\text{Cl}_3\text{O}_2$		Ac-d_6	142.1(C1) 144.5(C2) 118.6(C3) 122.9(C4) 120.5(C5) 119.6(C6)	80Knu
$\text{C}_6\text{H}_4\text{BrCl}$		CDCl_3	135.1(C1) 131.5(C2) 122.7(C3) 127.3(C4) 130.8(C5) 129.8(C6)	86Bro
$\text{C}_6\text{H}_4\text{BrF}$		C_6H_6	109.7(C1) 159.9(C2) 116.7(C3) 129.0(C4) 125.3(C5) 134.0(C6)	72Smi
$\text{C}_6\text{H}_4\text{BrF}$		CDCl_3	122.5(C1) 119.2(C2) 162.6(C3) 114.2(C4) 130.9(C5) 127.4(C6)	86Bro
$\text{C}_6\text{H}_4\text{BrF}$		Neat	117.5(C1) 133.5(C2/6) 117.8(C3/5) 163.3(C4)	72Miy
$\text{C}_6\text{H}_4\text{BrNO}_2$		CDCl_3 / DMSO-d_6	128.8(C1) 152.8(C2) 125.5(C3) 128.2(C4) 135.1(C5) 133.1(C6)	92Ras
$\text{C}_6\text{H}_4\text{BrNO}_2$		DMSO	123.5(C1) 127.1(C2) 107.3(C3) 123.5(C4) 132.7(C5) 138.5(C6)	71Miy
$\text{C}_6\text{H}_4\text{BrNO}_2$		CDCl_3	129.9(C1) 132.7(C2/6) 125.0(C3/5) 147.1(C4)	89Str

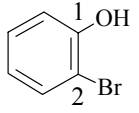
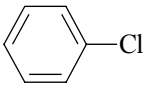
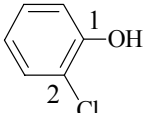
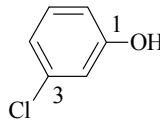
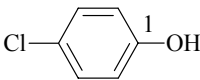
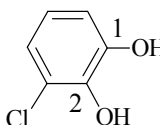
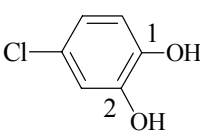
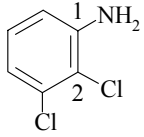
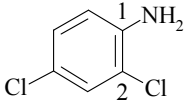
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_4\text{BrNO}_3$		DMSO	151.4(C1) 137.7(C2) 127.2(C3) 109.3(C4) 137.5(C5) 121.3(C6)	87Hut
$\text{C}_6\text{H}_4\text{Br}_2$		CDCl_3	124.6(C1/2) 133.4(C3/6) 128.2(C4/5)	85Tak
$\text{C}_6\text{H}_4\text{Br}_2$		CDCl_3	123.0(C1/3) 134.2(C2) 130.2(C4/6) 131.1(C5)	86Bro
$\text{C}_6\text{H}_4\text{Br}_2$		CDCl_3	121.0(C1/4) 133.1(C2/3/5/6)	80Bro
$\text{C}_6\text{H}_4\text{Br}_2\text{N}_2\text{O}_2$		DMSO-d_6	149.0(C1) 105.4(C2/6) 127.7(C3/5) 136.8(C4)	89Str
$\text{C}_6\text{H}_4\text{ClF}$		Ac-d_6	158.8(C1) 121.4(C2) 131.2(C3) 125.5(C4) 128.8(C5) 117.0(C6)	79Bre
$\text{C}_6\text{H}_4\text{ClF}$		CDCl_3	162.7(C1) 116.3(C2) 135.0(C3) 124.6(C4) 130.6(C5) 113.7(C6)	86Bro
$\text{C}_6\text{H}_4\text{ClF}$		Neat	129.6(C1) 130.1(C2/6) 116.8(C3/5) 161.8(C4)	72Miy
$\text{C}_6\text{H}_4\text{ClNO}$		Ac-d_6	142.7(C1) 130.6(C2/6) 122.8(C3/5) 164.8(C4)	79Cox
$\text{C}_6\text{H}_4\text{ClNOS}$		CDCl_3	141.2(C1) 128.4(C2/6) 129.5(C3/5) 136.2(C4)	76Kre
$\text{C}_6\text{H}_4\text{ClNO}_2$		CDCl_3 / DMSO-d_6	127.5(C1) 149.9(C2) 126.0(C3) 128.0(C4) 133.5 ^a (C5) 132.3 ^a (C6)	92Ras

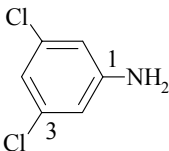
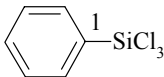
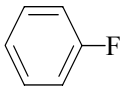
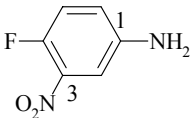
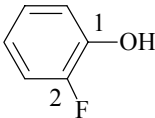
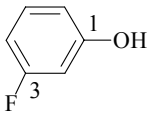
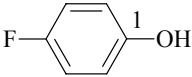
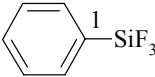
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_4\text{ClNO}_2$		DMSO	135.9(C1) 124.3(C2) 149.7(C3) 122.8(C4) 132.3(C5) 135.5(C6)	71Miy
$\text{C}_6\text{H}_4\text{ClNO}_3$		DMSO	151.2(C1) 137.2(C2) 124.5(C3) 122.5(C4) 134.9(C5) 120.9(C6)	87Hut
$\text{C}_6\text{H}_4\text{Cl}_2$		CDCl_3	132.6(C1/2) 130.5(C3/6) 127.7(C4/5)	72Jon
$\text{C}_6\text{H}_4\text{Cl}_2$		CDCl_3	135.0(C1/3) 128.7(C2) 126.9(C4/6) 130.4(C5)	86Bro
$\text{C}_6\text{H}_4\text{Cl}_2$		CDCl_3	132.5(C1/4) 129.8(C2/3/5/6)	80Bro
$\text{C}_6\text{H}_4\text{Cl}_2\text{N}_2\text{O}_2$		DMSO- d_6	147.4(C1) 116.7(C2/6) 124.0(C3/5) 135.4(C4)	89Str
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	152.9(C1) 119.2(C2) 132.8(C3) 122.3(C4) 128.2(C5) 114.6(C6)	80Ilc
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	150.3(C1) 120.6(C2) 128.7(C3) 125.8(C4) 128.7(C5) 117.3(C6)	80Ilc
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	152.0(C1) 118.5(C2) 129.7(C3) 121.8(C4) 133.9(C5) 116.8(C6)	80Ilc
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	148.1(C1) 121.3(C2/6) 128.5(C3/5) 121.3(C4)	80Ilc

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	154.6(C1) 117.7(C2) 133.1(C3) 124.4(C4) 131.0(C5) 115.4(C6)	80Ilc
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}$		CDCl_3	156.7(C1) 114.7(C2/6) 135.6(C3/5) 121.4(C4)	80Ilc
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}_2$		Ac-d_6	145.4(C1) 143.9(C2) 119.3(C3) 122.7(C4) 120.1(C5) 114.3(C6)	80Knu
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}_2$		Ac-d_6	147.4(C1) 141.6(C2) 121.0(C3) 119.8(C4) 123.7(C5) 114.4(C6)	80Knu
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}_2$		Ac-d_6	143.4(C1/2) 119.4(C3/6) 120.5(C4/5)	80Knu
$\text{C}_6\text{H}_4\text{Cl}_2\text{O}_2$		Ac-d_6	145.4(C1/2) 116.8(C3/6) 121.7(C4/5)	80Knu
$\text{C}_6\text{H}_4\text{Cl}_4\text{Si}$		n.r.	138.6(C1) 128.0(C2/6) 133.5(C3/5) 128.8(C4)	75Sch
$\text{C}_6\text{H}_4\text{FI}$		CDCl_3	161.5(C1) 81.2(C2) 139.3(C3) 125.6(C4) 129.9(C5) 115.6(C6)	96Rae
$\text{C}_6\text{H}_4\text{FI}$		Neat	163.9(C1) 118.8(C2/6) 140.1(C3/5) 90.0(C4)	72Miy
$\text{C}_6\text{H}_4\text{FNO}_2$		CDCl_3	155.5(C1) 137.2(C2) 126.1(C3) 124.7(C4) 135.8(C5) 118.5(C6)	96Rae

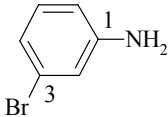
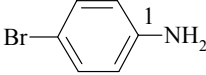
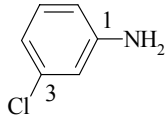
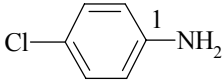
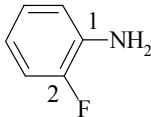
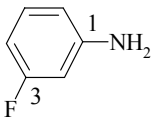
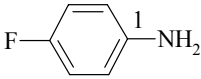
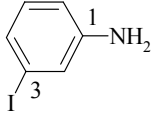
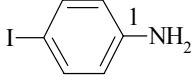
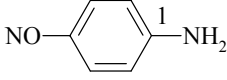
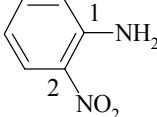
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_4\text{FNO}_2$		CDCl_3	162.3(C1) 111.3(C2) 149.2(C3) 119.4(C4) 130.7(C5) 121.8(C6)	86Bro
$\text{C}_6\text{H}_4\text{FNO}_3$		DMSO	148.9(C1) 136.2(C2) 111.5(C3) 153.9(C4) 122.8(C5) 120.6(C6)	87Hut
$\text{C}_6\text{H}_4\text{FNO}_3$		DMSO 318K	140.3(C1) 137.9(C2) 119.7(C3) 117.9(C4) 120.8(C5) 151.4(C6)	75Ste
$\text{C}_6\text{H}_4\text{FNO}_3$		DMSO 318K	154.0(C1) 132.4(C2) 127.3(C3) 106.3(C4) 164.9(C5) 104.8(C6)	75Ste
$\text{C}_6\text{H}_4\text{F}_2$		C_6H_{12}	151.1(C1/2) 117.6(C3/6) 124.6(C4/5)	72Smi
$\text{C}_6\text{H}_4\text{F}_2$		CDCl_3	163.1(C1/3) 104.0(C2) 111.2(C4/6) 130.6(C5)	86Bro
$\text{C}_6\text{H}_4\text{F}_2$		CDCl_3	159.1(C1/4) 116.5(C2/3/5/6) $^1J(\text{F}, \text{C1})=242.7$ $^4J(\text{F}, \text{C4})=3.7$	72Jon
$\text{C}_6\text{H}_4\text{FNO}_2$		Neat	166.2(C1) 116.5(C2/6) 126.4(C3/5) 144.8(C4)	72Miy
$\text{C}_6\text{H}_4\text{INO}_3$		DMSO	151.8(C1) 138.2(C2) 132.8(C3) 79.9(C4) 143.2(C5) 121.5(C6)	87Hut
$\text{C}_6\text{H}_4\text{I}_2\text{N}_2\text{O}_2$		DMSO- d_6	153.0(C1) 78.2(C2/6) 134.7(C3/5) 138.0(C4)	89Str
$\text{C}_6\text{H}_4\text{N}_2\text{O}_3$		Ac- d_6	164.2(C1) 122.2(C2/6) 126.4(C3/5) 159.1(C4)	79Cox

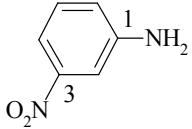
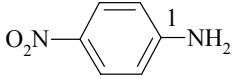
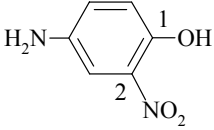
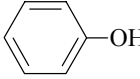
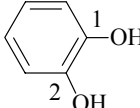
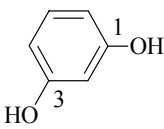
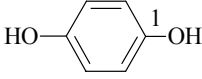
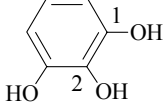
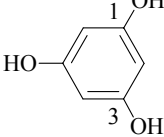
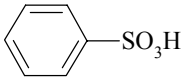
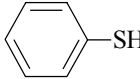
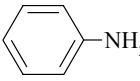
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_4\text{N}_2\text{O}_3\text{S}$		CDCl_3	146.9(C1) 127.9(C2/6) 125.5(C3/5) 148.0(C4)	76Kre
$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$		$\text{CDCl}_3/\text{DMSO-d}_6$	144.4(C1/2) 125.5(C3/6) 133.9(C4/5)	92Ras
$\text{C}_6\text{H}_4\text{N}_2\text{O}_4$		CDCl_3	148.4(C1/3) 119.1(C2) 128.9(C4/6) 130.7(C5)	86Bro
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$		CDCl_3	159.2(C1) 132.8(C2) 122.0(C3) 140.4(C4) 131.8(C5) 121.4(C6)	80Ilc
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$		CDCl_3	155.4(C1) 136.7(C2) 126.9(C3) 116.1 ^a (C4) 152.2(C5) 114.7 ^a (C6)	80Ilc
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$		CDCl_3	148.7(C1) 136.0(C2/6) 131.7(C3/5) 118.5(C4)	97Han
$\text{C}_6\text{H}_4\text{N}_2\text{O}_5$		DMSO	157.6(C1) 136.4(C2) 122.0(C3) 138.5(C4) 129.5(C5) 119.9(C6)	87Hut
$\text{C}_6\text{H}_5\text{Br}$		CDCl_3	122.4(C1) 131.4(C2/6) 129.9(C3/5) 126.7(C4)	81Bai
			$^1J(\text{C2},\text{H2})=165.8$ $^1J(\text{C3},\text{H3})=161.9$ $^1J(\text{C4},\text{H4})=161.6$ $^2J(\text{C1},\text{H2})=3.3$ $^2J(\text{C2},\text{H3})=1.4$ $^2J(\text{C3},\text{H2})=0.5$ $^2J(\text{C3},\text{H4})=1.6$ $^2J(\text{C4},\text{H3})=0.9$ $^3J(\text{C1},\text{H3})=11.2$ $^3J(\text{C2},\text{H4})=7.9$ $^3J(\text{C2},\text{H6})=5.3$ $^3J(\text{C3},\text{H5})=8.2$ $^3J(\text{C4},\text{H2})=7.4$ $^4J(\text{C1},\text{H4})=1.9$ $^4J(\text{C2},\text{H5})=1.2$ $^4J(\text{C3},\text{H6})=1.0$	72Tar
$\text{C}_6\text{H}_5\text{BrO}$		DMSO	156.8(C1) 117.6(C2/6) 132.1(C3/5) 110.1(C4)	87Hut

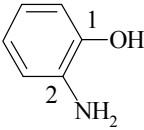
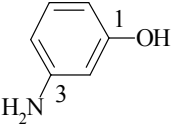
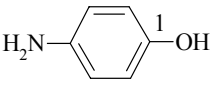
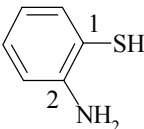
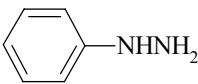
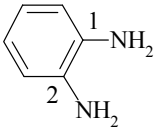
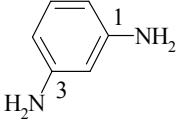
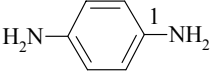
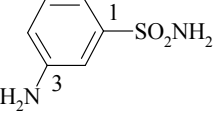
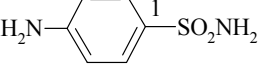
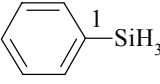
Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_5\text{BrO}$		DMSO	153.9(C1) 109.3(C2) 132.6(C3) 120.2(C4) 128.2(C5) 116.4(C6)	76Smi1
$\text{C}_6\text{H}_5\text{Cl}$		CDCl_3	134.2(C1) 128.6(C2/6) 129.6(C3/5) 126.4(C4) $^1J(\text{C2},\text{H2})=164.8$ $^1J(\text{C3},\text{H3})=161.2$ $^1J(\text{C4},\text{H4})=161.3$ $^2J(\text{C1},\text{H2})=3.4$ $^2J(\text{C2},\text{H3})=1.4$ $^2J(\text{C3},\text{H2})=0.3$ $^2J(\text{C3},\text{H4})=1.6$ $^2J(\text{C4},\text{H3})=0.9$ $^3J(\text{C1},\text{H3})=11.1$ $^3J(\text{C2},\text{H4})=7.9$ $^3J(\text{C2},\text{H6})=5.0$ $^3J(\text{C3},\text{H5})=8.2$ $^3J(\text{C4},\text{H2})=7.4$ $^4J(\text{C1},\text{H4})=2.0$ $^4J(\text{C2},\text{H5})=1.2$ $^4J(\text{C3},\text{H6})=0.9$	81Bai 72Tar
$\text{C}_6\text{H}_5\text{ClO}$		CDCl_3	151.8(C1) 120.3(C2) 129.2(C3) 121.5(C4) 128.5(C5) 116.5(C6)	80Ilc
$\text{C}_6\text{H}_5\text{ClO}$		CDCl_3	156.3(C1) 116.1(C2) 135.1(C3) 121.3(C4) 130.6(C5) 113.9(C6)	80Ilc
$\text{C}_6\text{H}_5\text{ClO}$		CDCl_3	154.1(C1) 116.8(C2/6) 129.7(C3/5) 125.9(C4)	80Ilc
$\text{C}_6\text{H}_5\text{ClO}_2$		Ac-d_6	146.8(C1) 142.2(C2) 120.5(C3) 120.7(C4) 120.3(C5) 114.4(C6)	80Knu
$\text{C}_6\text{H}_5\text{ClO}_2$		Ac-d_6	144.5(C1) 146.4(C2) 115.6(C3) 123.8(C4) 119.7(C5) 116.5(C6)	80Knu
$\text{C}_6\text{H}_5\text{Cl}_2\text{N}$		CDCl_3	144.7(C1) 117.5(C2) 133.2(C3) 119.5(C4) 127.5(C5) 113.6(C6) $^1J(\text{C4},\text{H4})=168.5$ $^1J(\text{C5},\text{H5})=161.7$ $^1J(\text{C6},\text{H6})=163.6$ $^3J(\text{C1},\text{H5})=9.3$ $^3J(\text{C2},\text{H4})=8.3$ $^3J(\text{C2},\text{H6})=8.8$ $^3J(\text{C3},\text{H5})=9.5$ $^3J(\text{C4},\text{H6})=8.4$ $^3J(\text{C6},\text{H4})=8.0$	77Ner
$\text{C}_6\text{H}_5\text{Cl}_2\text{N}$		CDCl_3	141.8(C1) 119.6(C2) 129.0(C3) 122.9(C4) 127.7(C5) 116.4(C6)	77Ner

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
			$^1J(\text{C3},\text{H3})=168.1$ $^1J(\text{C5},\text{H5})=165.1$ $^1J(\text{C6},\text{H6})=160$ $^3J(\text{C1},\text{H3})=6.2$ $^3J(\text{C1},\text{H5})=8.8$ $^3J(\text{C2},\text{H6})=8.8$ $^3J(\text{C3},\text{H5})=5.7$ $^3J(\text{C4},\text{H6})=12.0$ $^3J(\text{C5},\text{H3})=5.9$	
$\text{C}_6\text{H}_5\text{Cl}_2\text{N}$		CDCl_3	148.3(C1) 113.2(C2/6) 135.5(C3/5) 118.4(C4) $^1J(\text{C2},\text{H2})=160.1$ $^1J(\text{C4},\text{H4})=172.3$ $^3J(\text{C4},\text{H2})=4.9$ $^3J(\text{C6},\text{H2})=4.4$	77Ner
$\text{C}_6\text{H}_5\text{Cl}_3\text{Si}$		Neat	131.4(C1) 133.1(C2/6) 128.6(C3/5) 132.8(C4)	75Ngu
$\text{C}_6\text{H}_5\text{F}$		CDCl_3	163.0(C1) 115.3(C2/6) 130.0(C3/5) 124.0(C4)	81Bai
			$^1J(\text{F},\text{C1})=245.2$ $^2J(\text{F},\text{C2})=21.0$ $^3J(\text{F},\text{C3})=7.8$ $^4J(\text{F},\text{C4})=3.22$	76Che
			$^1J(\text{C2},\text{H2})=162.4$ $^1J(\text{C3},\text{H3})=160.9$ $^1J(\text{C4},\text{H4})=161.3$ $^2J(\text{C1},\text{H2})=4.9$ $^2J(\text{C2},\text{H3})=1.1$ $^2J(\text{C3},\text{H2})=0.5$ $^2J(\text{C3},\text{H4})=1.7$ $^2J(\text{C4},\text{H3})=0.8$ $^3J(\text{C1},\text{H3})=10.9$ $^3J(\text{C2},\text{H4})=8.3$ $^3J(\text{C2},\text{H6})=4.1$ $^3J(\text{C3},\text{H5})=9.0$ $^3J(\text{C4},\text{H2})=7.6$ $^4J(\text{C1},\text{H4})=1.8$ $^4J(\text{C2},\text{H5})=1.5$ $^4J(\text{C3},\text{H6})=0.8$	
$\text{C}_6\text{H}_5\text{FN}_2\text{O}_2$		DMSO 318K	145.5(C1) 107.9(C2) 136.6(C3) 145.5(C4) 117.9(C5) 120.0(C6)	75Ste
$\text{C}_6\text{H}_5\text{FO}$		CDCl_3	143.5(C1) 151.3(C2) 115.7(C3) 120.9(C4) 124.8(C5) 117.6(C6)	96Rae
$\text{C}_6\text{H}_5\text{FO}$		DMSO 318K	160.2(C1) 102.4(C2) 164.2(C3) 105.2(C4) 130.2(C5) 111.4(C6)	75Ste
$\text{C}_6\text{H}_5\text{FO}$		DMSO	153.8(C1) 116.3(C2/6) 115.8(C3/5) 155.7(C4)	87Hut
$\text{C}_6\text{H}_5\text{F}_3\text{Si}$		Neat	120.1(C1) 133.9(C2/6) 128.1(C3/5) 132.7(C4)	75Ngu

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_5\text{I}$		CDCl_3	94.3(C1) 137.2(C2/6) 130.0(C3/5) 127.2(C4)	81Bai
			$^1J(\text{C2},\text{H2})=165.7$ $^1J(\text{C3},\text{H3})=161.4$ $^1J(\text{C4},\text{H4})=161.0$ $^2J(\text{C1},\text{H2})=2.4$ $^2J(\text{C2},\text{H3})=1.6$ $^2J(\text{C3},\text{H2})=0.7$ $^2J(\text{C3},\text{H4})=1.4$ $^2J(\text{C4},\text{H3})=0.8$ $^3J(\text{C1},\text{H3})=10.7$ $^3J(\text{C2},\text{H4})=7.8$ $^3J(\text{C2},\text{H6})=6.0$ $^3J(\text{C3},\text{H5})=8.2$ $^3J(\text{C4},\text{H2})=7.4$ $^4J(\text{C1},\text{H4})=1.9$ $^4J(\text{C2},\text{H5})=1.3$ $^4J(\text{C3},\text{H6})=1.3$	72Tar
$\text{C}_6\text{H}_5\text{IO}$		DMSO	157.4(C1) 118.3(C2/6) 138.0(C3/5) 80.8(C4)	87Hut
$\text{C}_6\text{H}_5\text{IO}$		DMSO	155.5(C1) 86.1(C2) 138.7(C3) 122.7(C4) 76Smi1 130.3(C5) 115.8(C6)	
$\text{C}_6\text{H}_5\text{NO}$		Ac-d_6	166.8(C1) 121.1(C2/6) 130.2(C3/5) 136.6(C4)	79Cox
$\text{C}_6\text{H}_5\text{NOS}$		CDCl_3	142.7(C1) 127.1(C2/6) 129.1(C3/5) 130.4(C4)	76Kre
$\text{C}_6\text{H}_5\text{NO}_2$		CCl_4	148.2(C1) 123.2(C2/6) 129.1(C3/5) 134.2(C4)	89Bie
$\text{C}_6\text{H}_5\text{NO}_3$		CDCl_3	155.2(C1) 133.7(C2) 125.1(C3) 120.2(C4) 137.6(C5) 120.0(C6)	97Han
$\text{C}_6\text{H}_5\text{NO}_3$		CDCl_3	161.5(C1) 115.9(C2/6) 126.4(C3/5) 141.7(C4)	80Ilc
C_6H_6		Neat	128.4(C1-6)	72Nel
		CDCl_3	128.6(C1-6)	72Nel
		CCl_4	128.5(C1-6)	72Nel
		Ac	128.7(C1-6)	72Nel
			$^1J(\text{C1},\text{H1})=158.8$ $^2J(\text{C1},\text{H2})=1.1$ $^3J(\text{C1},\text{H3})=7.6$ $^4J(\text{C1},\text{H4})=1.2$	72Tar
		MeOH	128.5(C1-6)	72Nel
		CH_3COOH	128.6(C1-6)	72Nel

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
		CF ₃ COOH	128.6(C1-6)	72Nel
C ₆ H ₆ BrN		CDCl ₃	147.8(C1) 117.8(C2) 123.0(C3) 121.3(C4) 130.6(C5) 113.6(C6)	91Bud
C ₆ H ₆ BrN		CDCl ₃	145.4(C1) 116.7(C2/6) 132.0(C3/5) 110.2(C4)	91Bud
C ₆ H ₆ ClN		CDCl ₃	147.7(C1) 114.9(C2) 134.9(C3) 118.4(C4) 130.3(C5) 113.2(C6)	91Bud
C ₆ H ₆ ClN		CDCl ₃	145.0(C1) 116.2(C2/6) 129.1(C3/5) 123.2(C4)	91Bud
C ₆ H ₆ FN		CDCl ₃	134.5(C1) 151.7(C2) 115.2(C3) 118.6(C4) 124.4(C5) 116.9(C6)	96Rae
C ₆ H ₆ FN		CDCl ₃	148.6(C1) 102.0(C2) 163.9(C3) 104.8(C4) 130.5(C5) 110.8(C6) ¹ $J(\text{F}, \text{C}3)=242.6$ ² $J(\text{F}, \text{C}2)=24.8$ ² $J(\text{F}, \text{C}4)=21.4$ ³ $J(\text{F}, \text{C}1)=10.7$ ³ $J(\text{F}, \text{C}5)=10.0$	72Jon
C ₆ H ₆ FN		CDCl ₃	142.5(C1) 116.1(C2/6) 115.7(C3/5) 156.5(C4)	91Bud
C ₆ H ₆ IN		CDCl ₃	147.7(C1) 123.7(C2) 94.9(C3) 127.4(C4) 130.7(C5) 114.3(C6)	91Bud
C ₆ H ₆ IN		CDCl ₃	146.1(C1) 117.3(C2/6) 138.0(C3/5) 79.4(C4)	91Bud
C ₆ H ₆ N ₂ O		DMSO-d ₆	157.2(C1) 112.2(C2/6) 125.3(C3/5) 163.1(C4)	79Cox
C ₆ H ₆ N ₂ O ₂		CDCl ₃ / DMSO-d ₆	144.6(C1) 131.7(C2) 125.6(C3) 118.5(C4) 135.2(C5) 116.2(C6)	92Ras

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_6\text{N}_2\text{O}_2$		CDCl_3	147.6(C1) 109.1(C2) 149.4(C3) 113.2(C4) 130.0(C5) 120.7(C6)	91Bud
$\text{C}_6\text{H}_6\text{N}_2\text{O}_2$		CDCl_3	152.6(C1) 113.5(C2/6) 126.4(C3/5) 139.4(C4)	91Bud
$\text{C}_6\text{H}_6\text{N}_2\text{O}_3$		DMSO	144.5(C1) 135.6(C2) 107.4(C3) 141.9(C4) 124.3(C5) 120.2(C6)	87Hut
$\text{C}_6\text{H}_6\text{O}$		CCl_4	155.4(C1) 115.8(C2/6) 129.9(C3/5) 121.2(C4)	72Nel
$\text{C}_6\text{H}_6\text{O}_2$		Ac-d_6	145.6(C1/2) 116.0(C3/6) 120.7(C4/5)	78Nak
$\text{C}_6\text{H}_6\text{O}_2$		Ac-d_6	159.0(C1/3) 103.3(C2) 107.5(C4/6) 130.6(C5)	78Nak
$\text{C}_6\text{H}_6\text{O}_2$		Ac-d_6	150.8(C1/4) 116.5(C2/3/5/6)	78Nak
$\text{C}_6\text{H}_6\text{O}_3$		Ac-d_6	146.1(C1/3) 133.1(C2) 107.5(C4/6) 119.3(C5)	80Knu
$\text{C}_6\text{H}_6\text{O}_3$		Ac-d_6	159.5(C1/3/5) 94.8(C2/4/6)	80Knu
$\text{C}_6\text{H}_6\text{O}_3\text{S}$		H_2O	143.5(C1) 126.3(C2/6) 129.8(C3/5) 132.3(C4)	72Jon
$\text{C}_6\text{H}_6\text{S}$		CCl_4 317K	130.9(C1) 128.9(C2/6) 129.2(C3/5) 125.3(C4)	78Net
$\text{C}_6\text{H}_7\text{N}$		CCl_4	146.5(C1) 115.2(C2/6) 129.4(C3/5) 118.7(C4)	89Bie

Gross formula	Structure	Solvent	$\delta^{13}\text{C}$ [ppm] / J [Hz]	Ref.
$\text{C}_6\text{H}_7\text{NO}$		CDCl_3	145.8(C1) 137.8(C2) 116.3(C3) 121.4(C4) 118.7(C5) 116.5(C6)	86Bul
$\text{C}_6\text{H}_7\text{NO}$		CDCl_3	158.2(C1) 102.8(C2) 147.4(C3) 107.1(C4) 130.0(C5) 106.3(C6)	91Bud
$\text{C}_6\text{H}_7\text{NO}$		CDCl_3	150.0(C1) 116.7 ^a (C2/6) 116.1 ^a (C3/5) 138.5(C4)	91Bud
$\text{C}_6\text{H}_7\text{NS}$		CDCl_3	111.8(C1) 147.0(C2) 115.1(C3) 134.5(C4) 118.5(C5) 128.8(C6)	86Bul
$\text{C}_6\text{H}_8\text{N}_2$		CDCl_3	151.3(C1) 112.0(C2/6) 129.0(C3/5) 118.9(C4)	72Jon
$\text{C}_6\text{H}_8\text{N}_2$		CDCl_3	135.0(C1/2) 116.4(C3/6) 120.0(C4/5)	86Bul
$\text{C}_6\text{H}_8\text{N}_2$		CDCl_3	147.6(C1/3) 102.0(C2) 106.0(C4/6) 130.2(C5)	91Bud
$\text{C}_6\text{H}_8\text{N}_2$		CDCl_3	138.6(C1/4) 116.7(C2/3/5/6)	91Bud
$\text{C}_6\text{H}_8\text{N}_2\text{O}_2\text{S}$		CDCl_3 / DMSO-d_6	144.1(C1) 111.7(C2) 147.8(C3) 117.9(C4) 129.5(C5) 114.6(C6)	91Bud
$\text{C}_6\text{H}_8\text{N}_2\text{O}_2\text{S}$		CDCl_3 / DMSO-d_6	131.2(C1) 128.2(C2/6) 113.8(C3/5) 150.6(C4)	91Bud
$\text{C}_6\text{H}_8\text{Si}$		Neat	127.5(C1) 135.5(C2/6) 127.7(C3/5) 129.4(C4)	75Ngu