Additivity Parameters for 13

C Chemical Shifts in Substituted Benzenes*

Substituent	Ipso**	Ortho	Meta	Para
H	0.0	0.0	0.0	0.0
CH_3	8.9	0.7	-0.1	-2.9
C_2H_5	15.6	-0.4	0.0	-2.6
i-C_3H_7	20.2	-2.5	0.1	-2.4
t-C_4H_9	22.0	-3.4	-0.4	-3.1
$CH=CH_2$	9.5	-2.0	0.2	-0.5
C_6H_5	13.1	-1.1	0.4	-0.2
CF_3	2.6	-3.3	-0.3	3.2
OH	26.9	-12.7	1.4	-7.3
OCH_3	31.4	-14.4	1.0	-7.7
OC_2H_5	31.0	-13.7	1.1	-7.9
SCH_3	10.2	-1.8	0.4	-3.6
C(O)H	9.0	1.2	1.2	6.0

Substituent	Ipso**	Ortho	Meta	Para
C(O)OH	2.1	1.5	0.0	5.1
$C(O)CH_3$	9.1	0.1	0.0	4.2
CN	-15.4	3.6	0.6	3.9
NH_2	18.0	-13.3	0.9	-9.8
$NHC(O)CH_3$	11.1	-9.9	0.2	-5.6
$N(CH_3)_2$	22.6	-15.6	1.0	-11.5
NO_2	20.0	-4.8	0.9	5.8
F	34.8	-12.9	1.4	-4.5
Cl	6.2	0.4	1.3	-1.9
Br	-5.5	3.4	1.7	-1.6
I	-32.0	10.2	2.9	1.0
$Si(CH_3)_3$	13.4	4.4	-1.1	-1.1
$Sn(CH_3)_3$	13.1	7.2	-0.4	-0.4

* Ppm relative to internal benzene. In CCl_4, except for $CH=CH_2$ (neat), $N(CH_3)_2$ (neat), $Si(CH_3)_3$ (neat), and $Sn(CH_3)_3$ (neat). Chemical shift of benzene: 128.5 ppm relative to TMS.

** Ipso refers to the carbon atom bearing the substituent.

Reference: Levy, Lichter and Nelson, pps. 111-112; Breitmaier and Voelter, pps. 256-258.