Appendix 1: Data Section

Table 27.6.1: Ground State (GS) Spectroscopic Properties of Diatomic Molecules.[2-7]

Molecule	$\tilde{\nu}_e(cm^{-1})$	$\tilde{\nu}_e\chi_e(cm^{-1})$	$\tilde{B}_e(cm^{-1})$	$\tilde{\alpha}_e(cm^{-1})$	$\tilde{D}_e(cm^{-1})$	R_e(Å)	D_o(eV)	GS
$^{1}H^{1}H$	4401.21	121.34	60.853	3.062	0.0471	0.7414	4.4776	$^{1}\Sigma_g^+$
$^{7}Li^{1}H$	1405.498	23.168	7.51373	0.21639	$8.617x10^{-4}$	1.5957	2.429	$^{1}\Sigma_g^+$
$^{12}C^{1}H$	2860.75	64.44	14.460	0.536	$14.5x10^{-4}$	1.1199	3.46	$^{2}\Pi$
$^{14}N^{1}H$	3282.7	79.0	16.6679	0.6504	$17.1x10^{-4}$	1.0362	3.69	$^{3}\Sigma^-$
$^{1}H^{19}F$	4138.385	89.943	20.9537	0.7934	$21.51x10^{-4}$	0.91681	5.86	$^{1}\Sigma_g^+$
$^{1}H^{35}Cl$	2990.925	52.800	10.5933	0.3070	$5.32x10^{-4}$	1.27455	4.432	$^{1}\Sigma_g^+$
$^{7}Li^{7}Li$	351.407	2.583	0.67253	0.00705	$9.87x10^{-6}$	2.6729	1.06	$^{1}\Sigma_g^+$
$^{12}C^{16}O$	2169.756	13.288	1.93160	0.01751	$6.121x10^{-6}$	1.1283	11.108	$^{1}\Sigma_g^+$
$^{14}N^{14}N$	2358.6	14.324	1.99824	0.01732	$5.8x10^{-6}$	1.0977	9.756	$^{1}\Sigma_g^+$
$^{14}N^{16}O$	1904.135	14.088	1.70489	0.01754	$0.54x10^{-6}$	1.15077	6.497	$^{2}\Pi$
$^{16}O^{16}O$	1580.16	11.9513	1.4456	0.01593	$4.839x10^{-6}$	1.20752	5.126	$^{3}\Sigma_g^-$
$^{35}Cl^{35}Cl$	559.75	2.6943	0.2442	0.00152	$0.186x10^{-6}$	1.988	2.476	$^{1}\Sigma_g^+$

Table 27.8.2: Character Tables for Common Point Groups.

$C_s=C_h$	E	σ_h	h = 2	
A'	1	1	x, y, x^2, y^2, z^2, xy	R_z
A"	1	-1	z, yz, xz	R_x, R_y
$\Gamma_{x,y,z}$	3	1		

$C_i=S_2$	E	i	h = 2	
A_g	1	1	x^2, y^2, z^2, xy, xz, yz	R_x, R_y, R_z
A_u	1	-1	x, y, z	
$\Gamma_{x,y,z}$	3	-3		

C_{2v}	E	C_2	σ_v	σ_v'	h = 4	
A_1	1	1	1	1	z, z^2, x^2, y^2	
A_2	1	1	-1	-1	xy	R_z
B_1	1	-1	1	-1	y, yz	R_x
B_2	1	-1	-1	1	x, xz	R_y
$\Gamma_{x,y,z}$	3	-1	1	1		

C_{3v}	E	$2C_3$	$3\sigma_v$	h = 6	
A_1	1	1	1	z, z^2, x^2+y^2	
A_2	1	1	-1		R_z
E	2	-1	0	(x,y),(x^2-y^2,xy),(xz,yz)	(R_x,R_y)
$\Gamma_{x,y,z}$	3	0	1		

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$	h = 8	
A_1	1	1	1	1	1	z, z^2, x^z+y^2	
A_2	1	1	1	-1	-1		R_z
B_1	1	-1	1	1	-1	x^2-y^2	
B_2	1	-1	1	-1	1	xy	
E	2	0	-2	0	0	(x,y) (xz, yz)	(R_x, R_y)
$\Gamma_{x,y,z}$	3	1	-1	1	1		

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$	h = 10	α = 72°
A_1	1	1	1	1	z, z^2, x^2+y^2	
A_2	1	1	1	-1		R_z
E_1	2	2 cos α	2 cos 2α	0	(x, y) (xz, yz)	(R_x, R_y)
E_2	2	2 cos 2α	2 cos α	0	(xy, x^2-y^2)	
$\Gamma_{x,y,z}$	3	1+2 cos α	1+2 cos 2α	1		

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$	h = 12	
A_1	1	1	1	1	1	1	z, z^2, x^2+y^2	
A_2	1	1	1	1	-1	-1		R_z
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	(x,y) (xz, yz)	(R_x, R_y)
E_2	2	-1	-1	2	0	0	(xy, x^2-y^2)	
$\Gamma_{x,y,z}$	3	2	0	-1	1	1		

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	h = 4	
A_1	1	1	1	1	x^z, y^2, z^2	
B_1	1	1	-1	-1	z, xy	R_z
B_2	1	-1	1	-1	y, xz	R_y
B_3	1	-1	-1	1	x, yz	R_x
$\Gamma_{x,y,z}$	3	-1	-1	-1		

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	*i*	σ(xy)	σ(xz)	σ(yz)		
A_g	1	1	1	1	1	1	1	1	x^2,y^2,z^2	
B_{1g}	1	1	-1	-1	1	1	-1	-1	xy	R_z
B_{2g}	1	-1	1	-1	1	-1	1	-1	xz	R_y
B_{3g}	1	-1	-1	1	1	-1	-1	1	yz	R_x
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	
$\Gamma_{x,y,z}$	3	-1	-1	-1	-3	1	1	1		

D_{3h}	E	σ_h	$2C_3$	$2S_3$	$3C_2'$	$3\sigma_v$	h = 12	
A_1'	1	1	1	1	1	1	z^2, x^2+y^2	
A_2'	1	1	1	1	-1	-1		R_z
A_1''	1	-1	1	-1	1	-1		
A_2''	1	-1	1	-1	-1	1	z	
E'	2	2	-1	-1	0	0	(x, y),(xy, x^2–y^2)	
E''	2	-2	-1	1	0	0	(xz, yz)	(R_x,R_y)
$\Gamma_{x,y,z}$	3	0	-1	1	-2	1		

T_d	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$	h = 24	
A_1	1	1	1	1	1	$x^2+y^2+z^2$	
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0	($3z^2$–r^2, x^2–y^2)	
T_1	3	0	-1	-1	1		(R_x,R_y,R_z)
T_2	3	0	-1	1	-1	(x, y, z),(xy, xz, yz)	
$\Gamma_{x,y,z}$	3	0	-1	1	-1		

Tabel 29.1.2: ^{1}H Chemical Shifts of Methyl, Methylene, and Methine Groups.[1-3]

	Methyl protons	δ_H	Methylene protons	δ_H	Methine protons	δ_H
C	CH_3–R	0.9	R–CH_2–R	1.4	>CH–R	1.5
	CH_3–C–C=C	1.1	R–CH_2–C–C=C	1.7	>CH–C–C=C	1.8
	CH_3–C–O	1.3	R–CH_2–C–O	1.9	>CH–C–O	2.0
	CH_3–C–N	1.1	R–CH_2–C–N	1.4	>CH–C–N	1.8
	CH_3–C–NO_2	1.6	R–CH_2–C–NO_2	2.1		
	CH_3–C=C	1.6	R–CH_2–C=C	2.3	>CH–C=C	2.6
	CH_3–Ar	2.3	R–CH_2–Ar	2.7	>CH–Ar	3.0
	CH_3–C=CC=O	2.0	R–CH_2–C=CC=O	2.4	>CH–C=CC=O	2.7
	C=C(CH_3)–C=O	1.8	C=C(CH_2–R)–C=O	2.4	C=C(CH<)–C=O	2.8
	CH_3–C≡C	1.8	R–CH_2–C≡C	2.2	>CH–C≡C	2.6
	CH_3–C(=O)–R	2.2	R–CH_2-C(=O)–R	2.4	>CH–C(=O)–R	2.7
	CH_3–C(=O)–Ar	2.6	R–CH_2-C(=O)–Ar	2.9	>CH–C(=O)–Ar	3.3
	CH_3–C(=O)–OR	2.0	R–CH_2-C(=O)–OR	2.2	>CH–C(=O)–OR	2.5
	CH_3–C(=O)–OAr	2.4	R–CH_2-C(=O)–OAr	2.7	>CH–C(=O)–OAr	2.7
	CH_3–C(=O)–N	2.0	R–CH_2-C(=O)–N	2.2	>CH–C(=O)–N	2.4
		2.0	R–CH_2–C≡N	2.3	>CH–C≡N	2.7
N	CH_3–N	2.3	R–CH_2–N	2.5	>CH–N	2.8
	CH_3–N–Ar	3.0	R–CH_2–N–Ar	3.1	>CH–N–Ar	3.6
	CH_3-N–C(=O)–R	2.9	R–CH_2–N–C(=O)–R	3.2	>CH–N–C(=O)–R	4.0
	CH_3–N^+	3.3	R–CH_2–N^+	3.3		
			R–CH_2–NO_2	4.4	>CH–NO_2	4.7
O			R–CH_2–OH	3.6	>CH–OH	3.9
	CH_3–OR	3.3	R–CH_2–OR	3.4	>CH–OR	3.7
	CH_3–O–C=C	3.8	R–CH_2–O–C=C	3.7	>CH–O–C=C	4.2
	CH_3–O–Ar	3.8	R–CH_2–O–Ar	4.3	>CH–O–Ar	4.5
	CH_3–O–C(=O)–R	3.7	R–CH_2–O–C(=O)–R	4.1	>CH–O–C(=O)–R	4.8
			RO–CH_2–OR	4.8	R–O–CH–OR	4.7
X			R–CH_2–F	4.4		
			R–CH_2–Cl	3.6	>CH–Cl	4.2
			R–CH_2–Br	3.5	>CH–Br	4.3
			R–CH_2–I	3.2	>CH–I	4.3
	CH_3–Si	0.0	R–CH_2–Si	0.5	>CH–Si	1.2
	CH_3–S	2.1	R–CH_2–S	2.4	>CH–S	3.2
	CH_3–S(=O)R	2.5	R–CH_2–S(=O)R	3.0		
	CH_3–S(O_2)R	2.8	R–CH_2–S(O_2)R	3.0		
	CH_3–S(O_2)O–R	3.2				
	CH_3–OS(O_2)–R	3.9	R–CH_2–OS(O_2)–R	4.3	>CH–OS(O_2)–R	4.7
			RS–CH_2–SR	3.8	RS–CH–SR	4.1

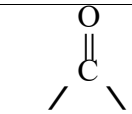
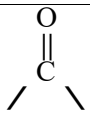
R = alkyl group. Typical uncertainty is ±0.3 ppm for methyl and methylene and ±0.5 ppm for methine unless electronic or anisotropic effects from other groups are strong.

1. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry. 4th Ed.*, McGraw Hill, London, UK, 1987, Table 3.17.

2. W. Hull, S. Krause, S. Kuhn, G. Schneider, C. Steinbeck, "Predict," *NMRShiftDB2*, Universität zu Köln, http://nmrshiftdb.nmr.uni-koeln.de/, last accessed 8/2/2016.

3. *SDBSWeb*, National Institute of Advanced Industrial Science and Technology, http://sdbs.db.aist.go.jp, last access 8/2/2016.

Table 29.1.4: ^{13}C Chemical Shifts of Carbonyl Carbons.[1-3]

					
R_1	R_2	δ_C	R_1	R_2	δ_C
Me–	–H	199.7	Me–	–OH	178.1
Et–	–H	206.0	Et–	–OH	180.4
Pr^n–	–H	202.8	Pr^n–	–OH	180.7
Pr^i–	–H	204.0	Pr^i–	–OH	184.1
Bu^n–	–H	202.8	Bu^n–	–OH	180.9
Bu^t–	–H	205.8	Bu^t–	–OH	185.9
CH_2=CH–	–H	192.4	CH_2=CH–	–OH	171.7
Ph–	–H	192.0	Ph–	–OH	172.6
Me–	–Me	206.0	H–	–OEt	161.4
Et–	–Me	207.6	Me–	–OMe	170.7
Pr^n–	–Me	208.9	Me–	–OEt	171.1
Pr^i–	–Me	211.8	Et–	–OMe	173.3
Bu^n–	–Me	209.0	Pr^n–	–OMe	175.7
Bu^t–	–Me	213.5	Pr^i–	–OMe	175.7
$HOCH_2$–	–Me	208.2	Bu^n–	–OMe	174.2
$ClCH_2$–	–Me	200.7	Bu^t–	–OMe	178.9
Cl_2CH–	–Me	193.6	CH_2=CH–	–OMe	165.5
Cl_3C–	–Me	186.3	Ph–	–OMe	166.8
CH_2=CH–	–Me	197.2	–	$(CH_2)_3O$ –	177.9
Ph–	–Me	197.6	–	$(CH_2)_4O$ –	175.2
Ph–	–Et	200.0	Me–	$–NH_2$	173.4
Ph–	–Ph	196.5	Et–	$–NH_2$	174.3
–	$(CH_2)_3$ –	208.2	CH_2=CH–	$–NH_2$	168.3
–	$(CH_2)_4$ –	213.9	Ph–	$–NH_2$	169.7
–	$(CH_2)_5$ –	208.8	Ph–	$–N(CH_3)_2$	171.6
–	$(CH_2)_6$ –	211.7	–	$(CH_2)_3NH$ –	179.4
$–CH_2CH_2CH$=CH–		209.0	–	$(CH_2)_4NH$ –	173.0
$–CH_2$=CH-CH=CH–		200.0	Me–	–OAc	167.3
$–CH_2CH_2CH_2CH$=CH–		198.0	Ph–	–OAc	162.8
			Me–	–Cl	170.3
			Et–	–Cl	174.7
			CH_2=CH–	–Cl	165.6
			Ph–	–Cl	168.3

1. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry. 4th Ed.*, McGraw Hill, London, UK, 1987, Table 3.13.
2. W. Hull, S. Krause, S. Kuhn, G. Schneider, C. Steinbeck, *NMRShiftDB2*, Universität zu Köln, http://nmrshiftdb.nmr.uni-koeln.de/, last accessed 8/2/2016.
3. *SDBSWeb*, National Institute of Advanced Industrial Science and Technology, http://sdbs.db.aist.go.jp, last accessed 8/2/2016.

Table 30.5.1: Atomic Energies in Hartrees (au) using *Ab Initio* Methods.[*(DS)]

Atom	HF/6-31G*	MP2/6-311G*	B3LYP/6-311G*	B3LYP/6-311+G*	B3LYP/cc-pVTZ
H	-0.4982329	-0.4998098	-0.5021559	-0.5021559	-0.5021563
Li	-7.4313723	-7.4320264	-7.4912968	-7.4913333	-7.4920159
Be	-14.5669444	-14.5985691	-14.6711842	-14.6713141	-14.6724455
B	-24.5220372	-24.5693278	-24.6618695	-24.6624669	-24.6637586
C	-37.6808603	-37.7450232	-37.8559888	-37.8572669	-37.8585746
N	-54.3854425	-54.4750512	-54.5985435	-54.6007232	-54.601781
O	-74.7839336	-74.9181455	-75.0853748	-75.0898713	-75.0918572
F	-99.3649569	-99.5541705	-99.7538101	-99.7605798	-99.7628675
Na	-161.841435	-161.845926	-162.286694	-162.286844	-162.296912
Mg	-199.5956109	-199.606556	-200.093098	-200.0932688	-200.0976386
Si	-288.8317857	-288.8921959	-289.393806	-289.3941537	-289.3963273
P	-340.6902044	-340.7671703	-341.2804859	-341.281716	-341.2858577
S	-397.4759577	-397.5807253	-398.1320492	-398.1330364	-398.1386911
Cl	-459.4479641	-459.5851374	-460.1661563	-460.1668773	-460.1746898

* SCF atom energies are identical at the "*" and "**" levels, or equivalently at the (d) and (d,p) levels.

Integral Table (a, b = constants; n, m = integers)

$\int u\,dv = uv - \int v\,du$ $\qquad \int x^n\,dx = x^{n+1}/(n+1)$ $\qquad \int \ln x\,dx = x\ln x - x$

$$\int \frac{dx}{a+bx} = \frac{1}{b}\ln(a+bx) \qquad \int \frac{x\,dx}{a+bx} = \frac{1}{b^2}[a+bx-a\ln(a+bx)]$$

$$\int \frac{dx}{x(a+bx)} = \frac{1}{a}\ln\left(\frac{x}{a+bx}\right) \qquad \int \frac{dx}{(a+bx)(a'+b'x)} = \frac{1}{ab'-a'b}\ln\left(\frac{a'+b'x}{a+bx}\right)$$

$$\int \frac{dx}{(a+bx)^2(a'+b'x)} = \frac{1}{ab'-a'b}\left[\frac{1}{a+bx} + \frac{b'}{ab'-a'b}\ln\left(\frac{a'+b'x}{a+bx}\right)\right]$$

Gaussian Functions

$$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2} \qquad \int_0^\infty x\,e^{-ax^2}\,dx = \frac{1}{2a}$$

$$\int_0^\infty x^2 e^{-ax^2}\,dx = \frac{1}{4a}\left(\frac{\pi}{a}\right)^{1/2} \qquad \int_0^\infty x^3 e^{-ax^2}\,dx = \frac{1}{2a^2}$$

$$\int_0^\infty x^4 e^{-ax^2}\,dx = \frac{3}{8a^2}\left(\frac{\pi}{a}\right)^{1/2} \qquad \int_0^\infty x^5 e^{-ax^2}\,dx = \frac{1}{a^3}$$

$$\int_0^\infty x^{2n} e^{-ax^2}\,dx = \frac{1\cdot3\cdot5\cdots(2n-1)}{2^{n+1}a^n}\left(\frac{\pi}{a}\right)^{1/2} \qquad \int_0^\infty x^{2n+1} e^{-ax^2}\,dx = \frac{n!}{2}\left(\frac{1}{a^{n+1}}\right)$$

$$\int_0^\infty e^{-x^2/2\sigma_x^2}\,dx = \tfrac{1}{2}(2\pi)^{1/2}\sigma_x \qquad \int_0^\infty x^2 e^{-x^2/2\sigma_x^2}\,dx = \frac{2\sigma_x^2}{4}(2\pi)^{1/2}\sigma_x$$

$$\frac{2}{\sqrt{\pi}}\int_0^t e^{-y^2}\,dy = \mathrm{erf}(t) \qquad \frac{1}{\sqrt{2\pi}}\int_0^z e^{-x^2/2}\,dx = \tfrac{1}{2}\,\mathrm{erf}(z/\sqrt{2})$$

$$\frac{1}{\sigma_x\sqrt{2\pi}}\int_0^{x_c} e^{-x^2/2\sigma_x^2}\,dx = \tfrac{1}{2}\,\mathrm{erf}\left(\frac{x_c}{\sigma_x\sqrt{2}}\right) \qquad \int_0^{x_c} e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{2}\,\mathrm{erf}(\sqrt{a}\,x_c)$$

z	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1.0	1.64485	2.0
$t = z/\sqrt{2}$	0.07071	0.14142	0.21213	0.28284	0.35355	0.42426	0.56569	0.70711	1.16309	1.41421
erf(t)	0.07966	0.15852	0.23582	0.31084	0.38292	0.45149	0.57629	0.68269	0.90000	0.95450

Exponential Functions ($a > 0$)

$$\int_0^\infty x^{-1/2} e^{-ax}\,dx = \sqrt{\pi}/a^{1/2}$$

$$\int_0^\infty x^{1/2} e^{-ax}\,dx = \sqrt{\pi}/(2a^{3/2})$$

$$\int x^n e^{-ax}\,dx = -\frac{x^n e^{-ax}}{a} + \frac{n}{a}\int x^{n-1} e^{-ax}\,dx \qquad \int_0^\infty x^n e^{-ax}\,dx = n!/a^{n+1}$$

$$\int e^{-ax}\,dx = -\frac{e^{-ax}}{a} \qquad \int_0^\infty e^{-ax}\,dx = 1/a$$

$$\int x\,e^{-ax}\,dx = -\frac{x\,e^{-ax}}{a} - \frac{e^{-ax}}{a^2} \qquad \int_0^\infty x\,e^{-ax}\,dx = 1/a^2$$

$$\int x^2 e^{-ax}\,dx = -\frac{x^2 e^{-ax}}{a} - \frac{2x\,e^{-ax}}{a^2} - \frac{2\,e^{-ax}}{a^3} \qquad \int_0^\infty x^2 e^{-ax}\,dx = 2/a^3$$

$$\int x^3 e^{-ax}\,dx = -\frac{x^3 e^{-ax}}{a} - \frac{3x^2 e^{-ax}}{a^2} - \frac{6x\,e^{-ax}}{a^3} - \frac{6\,e^{-ax}}{a^4} \qquad \int_0^\infty x^3 e^{-ax}\,dx = 6/a^4$$

Triginometric Functions

$\int \cos x\,dx = \sin x$ $\qquad \int_0^\pi \cos x\,dx = 0$

$\int \sin x\,dx = -\cos x$ $\qquad \int_0^\pi \sin x\,dx = 2$