Spectroscopically determined properties of selected diatomic molecules in the ground electronic state.[a,b]

(a. From M. Karplus, R. N. Porter, *Atoms and Molecules,* W. A. Benjamin, Menlo Park, CA, 1970. Table 7.3.)

Molecule	$\tilde{\nu}_e(cm^{-1})$	$\tilde{\nu}_e\chi_e(cm^{-1})$	$\tilde{B}_e(cm^{-1})$	$\tilde{\alpha}_e(cm^{-1})$	$\tilde{D}_e(cm^{-1})$	$R_e(\text{Å})$	$D_o(eV)$	Ground state
$C^{12}H^1$	2861.6	64.3	14.457	0.534	14.5×10^{-4}	1.1198	3.47	$^2\Pi$
$Cl^{35}Cl^{35}$	564.9	4.0	0.2438	0.0017	---	1.988	2.475	$^1\Sigma_g^+$
$C^{12}O^{16}$	2170.21	13.461	1.9314	0.01749	6.43×10^{-6}	1.1282	11.108	$^1\Sigma^+$
H^1H^1	4395.2	117.91	60.81	2.993	0.0464_8	0.7417	4.4763	$^1\Sigma_g^+$
H^1Cl^{35}	2989.74	52.05	10.5909	0.3019	5.32×10^{-4}	1.27460	4.430	$^1\Sigma^+$
Li^7Li^7	351.44	2.592	0.6727	0.00704	$9.8_6 \times 10^{-6}$	2.673	1.03	$^1\Sigma_g^+$
$N^{14}N^{14}$	2359.61	14.456	2.010	0.0187	5.8×10^{-6}	1.094	9.756	$^1\Sigma_g^+$
$N^{14}O^{16}$	1904.03	13.97	1.7046	0.0178	$\sim5 \times 10^{-6}$	1.1508	6.49	$^2\Pi$
$O^{16}O^{16}$	1580.361	12.0730	1.44567	0.01579	$4.95_7 \times 10^{-6}$	1.20740	5.080	$^3\Sigma_g^-$
$H^1 F^{19}$	4138.32	89.88	20.9557	0.798	2.151×10^{-3}	0.91680_8	5.869	$^1\Sigma^+$

[b]From G.Herzberg, Spectra of Diatomic Molecules (Van Nostrand, Princeton, NJ 1950); the data for many other molecules are also listed in this volume.

$\tilde{\nu}_e(cm^{-1})$ 	fundamental vibration frequency: $h\nu_e = hc\tilde{\nu}_e$ and the directly observed $h\nu_o = hc\tilde{\nu}_e - 2hc\tilde{\nu}_e\chi_e$

$\tilde{\nu}_e\chi_e(cm^{-1})$ 	anharmonicity: $E_\upsilon = h\nu_e (\upsilon + 1/2) - hc\tilde{\nu}_e\chi_e (\upsilon + 1/2)^2$

$\tilde{B}_e(cm^{-1})$ 	rotation constant: $\tilde{B}_e = \dfrac{\hbar}{4\pi\mu R_e^2 c}$

$\tilde{\alpha}_e(cm^{-1})$ 	vibration-rotation interaction: Coreolis constant: $\tilde{B}_\upsilon = \tilde{B}_e - \tilde{\alpha}_e (\upsilon + 1/2)$

$\tilde{D}_e(cm^{-1})$ 	centrifugal distortion: $\tilde{F}_J = \tilde{B}_e J(J+1) - \tilde{D}_e [J(J+1)]^2$

$R_e(\text{Å})$ equilibrium bond length from $\tilde{B}_e$; compare with R_o, vibrationally averaged bond length

$D_o(eV)$ 	dissociation energy, $D_e = D_o + 1/2\, h\nu_e - 1/4\, hc\, \tilde{\nu}_e\chi_e$ 	or

in cm^{-1}: 	$\tilde{D}_e = \tilde{D}_o + 1/2\, \tilde{\nu}_e - 1/4\, \tilde{\nu}_e\chi_e$ (but don't confuse with centrifugal distortion)