FORCE CONSTANTS FOR BOND STRETCHING

Representative force constants (f) for stretching of chemical bonds are listed in this table. Except where noted, all force constants are derived from values of the harmonic vibrational frequencies ω_e. Values derived from the observed vibrational fundamentals ν, which are noted by a, are lower than the harmonic force constants, typically by 2 to 3% in the case of heavy atoms (often by 5 to 10% if one of the atoms is hydrogen). Values are given in the SI unit newton per centimeter (N/cm), which is identical to the commonly used cgs unit mdyn/Å.

References

1. Huber, K. P., and Herzberg, G., *Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules*, Van Nostrand Reinhold, New York, 1979.
2. Shimanouchi, T., The Molecular Force Field, in Eyring, H., Henderson, D., and Yost, W., Eds., *Physical Chemistry: An Advanced Treatise*, Vol. IV, Academic Press, New York, 1970.
3. Tasumi, M., and Nakata, M., *Pure and Appl. Chem.*, 57, 121—147, 1985.

Bond	Molecule	f/(N/cm)	Note
H-H	H_2	5.75	
Be-H	BeH	2.27	
B-H	BH	3.05	
C-H	CH	4.48	
	CH_4	5.44	b
	C_2H_6	4.83	a,b,c
	CH_3CN	5.33	b
	CH_3Cl	5.02	a,b,c
	$CCl_2{=}CH_2$	5.57	b
	HCN	6.22	
N-H	NH	5.97	
O-H	OH	7.80	
	H_2O	8.45	
P-H	PH	3.22	
S-H	SH	4.23	
	H_2S	4.28	
F-H	HF	9.66	
Cl-H	HCl	5.16	
Br-H	HBr	4.12	
I-H	HI	3.14	
Li-H	LiH	1.03	
Na-H	NaH	0.78	
K-H	KH	0.56	
Rb-H	RbH	0.52	
Cs-H	CsH	0.47	
C-C	C_2	12.16	
	$CCl_2{=}CH_2$	8.43	
	C_2H_6	4.50	a,c
	CH_3CN	5.16	
C-F	CF	7.42	
	CH_3F	5.71	a,c
C-Cl	CCl	3.95	
	CH_3Cl	3.44	a,c
	$CCl_2{=}CH_2$	4.02	b
C-Br	CH_3Br	2.89	a,c
C-I	CH_3I	2.34	a,c
C-O	CO	19.02	
	CO_2	16.00	
	OCS	16.14	
	CH_3OH	5.42	a,c
C-S	CS	8.49	
	CS_2	7.88	
	OCS	7.44	
C-N	CN	16.29	
	HCN	18.78	
	CH_3CN	18.33	
	CH_3NH_2	5.12	a,c
C-P	CP	7.83	
Si-Si	Si_2	2.15	
Si-O	SiO	9.24	
Si-F	SiF	4.90	
Si-Cl	SiCl	2.63	
N-N	N_2	22.95	
	N_2O	18.72	
N-O	NO	15.95	
	N_2O	11.70	
P-P	P_2	5.56	
P-O	PO	9.45	
O-O	O_2	11.77	
	O_3	5.74	a
S-O	SO	8.30	
	SO_2	10.33	a
S-S	S_2	4.96	
F-F	F_2	4.70	
Cl-F	ClF	4.48	
Br-F	BrF	4.06	
Cl-Cl	Cl_2	3.23	
Br-Cl	BrCl	2.82	
Br-Br	Br_2	2.46	
I-I	I_2	1.72	
Li-Li	Li_2	0.26	
Li-Na	LiNa	0.21	
Na-Na	Na_2	0.17	
Li-F	LiF	2.50	
Li-Cl	LiCl	1.43	
Li-Br	LiBr	1.20	
Li-I	LiI	0.97	
Na-F	NaF	1.76	
Na-Cl	NaCl	1.09	
Na-Br	NaBr	0.94	
Na-I	NaI	0.76	
Be-O	BeO	7.51	
Mg-O	MgO	3.48	
Ca-O	CaO	3.61	

[a] Derived from fundamental frequency, without anharmonicity correction.
[b] Average of symmetric and antisymmetric (or degenerate) modes.
[c] Calculated from Local Symmetry Force Field (see Reference 2).