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

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