

## CHARACTERISTIC BOND LENGTHS IN FREE MOLECULES

This is a summary of typical bond lengths in gas-phase molecules. The value given for each bond is near the mid-range of values found in simple molecules. Bond lengths usually vary by 1 or 2%, and often by more, depending on the nature of the other bonds attached to the two atoms in question. References 1 and 2 give bond lengths in individual gas-phase molecules, as determined by spectroscopic and electron diffraction methods.

All bond distances are given in Å (1 Å = 10<sup>-10</sup> m).

### References

1. "Bond Lengths and Angles in Gas-Phase Molecules", *CRC Handbook of Chemistry and Physics*, 86th Edition, 2005, p. 9-19.
2. Harmony, M. D., Laurie, V. W., Kuczkowski, R. L., Schwendeman, R. H., Ramsay, D. A., Lovas, F. J., Lafferty, W. J., and Maki, A. G., Molecular structure of gas-phase polyatomic molecules determined by spectroscopic methods, *J. Phys. Chem. Ref. Data* 8, 619, 1979.
3. Lide, D. R., "A survey of carbon-carbon bond lengths", *Tetrahedron* 17, 125, 1962.

### A. Characteristic lengths of single bonds.

	As	Br	C	Cl	F	Ge	H	I	N	O	P	S	Sb	Se	Si
As	2.10														
Br	2.32	2.28													
C	1.96	1.94	1.53												
Cl	2.17	2.14	1.79	1.99											
F	1.71	1.76	1.39	1.63	1.41										
Ge		2.30	1.95	2.15	1.73	2.40									
H	1.51	1.41	1.09	1.28	0.92	1.53	0.74								
I		2.47	2.13	2.32	1.91	2.51	1.61	2.67							
N			1.46	1.90	1.37		1.02		1.45						
O				1.42	1.70	1.42		0.96		1.43	1.48				
P		2.22	1.85	2.04	1.57		1.42		1.65		2.25				
S		2.24	1.82	2.05	1.56		1.34					2.00			
Sb				2.33			1.70								
Se					1.95		1.71		1.47				2.33		
Si		2.21	1.87	2.05	1.58		1.48	2.44		1.63		2.14		2.33	
Sn			2.14	2.28			1.71	2.67							
Te						1.82	1.66								

### B. Lengths of multiple bonds (non-ring molecules).

C=C	1.34
C≡C	1.20
C=N	1.21
C≡N	1.16
C=O	1.21
C=S	1.61
N=N	1.24
N≡N	1.13
N=O	1.18
O=O	1.21

### C. Effect of environment on carbon-carbon single bonds (other single bonds not shown). From Reference 3.

Configuration	C–C length	Examples of molecules
C–C	1.526	$\text{H}_3\text{C}-\text{CH}_3$
C–C=	1.501	$\text{H}_3\text{C}-\text{CH}=\text{CH}_2$
C–C≡	1.459	$\text{H}_3\text{C}-\text{C}\equiv\text{CH}$
=C–C=	1.467	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$
≡C–C=	1.445	$\text{HC}\equiv\text{C}-\text{CH}=\text{CH}_2$
≡C–C≡	1.378	$\text{HC}\equiv\text{C}-\text{C}\equiv\text{CH}$

### D. Some metal–carbon bond lengths in gas-phase molecules.

Al–C	1.96	Bi–C	2.26	Pb–C	2.24
B–C	1.58	Cd–C	2.11	Sn–C	2.14
Be–C	1.70	Hg–C	2.08	Zn–C	1.93