

Common Elements and Their Isotopes

Element	Symbol	Exact Mass (μ)	Relative Abundance (%)
Hydrogen	^1H	1.007825037	100.0%
Deuterium	^2H or D	2.014101787	0.015%
Carbon 12	^{12}C	12.00000	98.9%
Carbon 13	^{13}C	13.003354	1.11%
Nitrogen 14	^{14}N	14.003074	99.6%
Nitrogen 15	^{15}N	15.00011	0.36%
Oxygen 16	^{16}O	15.99491464	99.8%
Oxygen 17	^{17}O	16.9991306	0.40%
Oxygen 18	^{18}O	17.99915939	0.200%
Fluorine	^{19}F	18.998405	100.0%
Sodium	^{23}Na	22.9897697	100.0%
Silicon 28	^{28}Si	27.9769284	92.2%
Silicon 29	^{29}Si	28.9764964	4.67%
Silicon 30	^{30}Si	29.9737717	3.1%
Phosphorus	^{31}P	30.9737634	100%
Sulfur 32	^{32}S	31.972074	95%
Sulfur 33	^{33}S	32.9707	0.76%
Sulfur 34	^{34}S	33.96838	4.22%
Sulfur 36	^{36}S	35.96676	0.20%
Chlorine 35	^{35}Cl	34.968854	75.8%
Chlorine 37	^{37}Cl	36.965896	24.2%



Amino Acids

Name	One Letter Symbol	Three Letter Symbol	Composition	Monoisotopic Residue Mass	Average Residue Mass
Glycine	G	Gly	C ₂ H ₅ N ₂ O ₂	57.02146	57.05192
Alanine	A	Ala	C ₃ H ₇ NO	71.03711	71.0788
Serine	S	Ser	C ₃ H ₅ NO ₂	87.03203	87.0782
Proline	P	Pro	C ₅ H ₇ NO	97.05276	97.11668
Valine	V	Val	C ₆ H ₉ NO	99.06841	99.13256
Threonine	T	Thr	C ₄ H ₇ NO ₂	101.04768	101.10508
Cysteine	C	Cys	C ₃ H ₅ NOS	103.00919	103.1448
Isoleucine	I	Ile	C ₆ H ₁₁ NO	113.08406	113.15944
Leucine	L	Leu	C ₆ H ₁₁ NO	113.08406	113.15944
Asparagine	N	Asn	C ₄ H ₆ N ₂ O ₂	114.04293	114.10384
Aspartic Acid	D	Asp	C ₄ H ₅ NO ₃	115.02694	115.0886
Glutamine	Q	Gln	C ₃ H ₅ N ₁ O ₇	128.05858	128.13072
Lysine	K	Lys	C ₆ H ₁₂ N ₂ O	128.09496	128.17408
Glutamic Acid	E	Glu	C ₅ H ₇ NO ₃	129.04259	129.11548
Methionine	M	Met	C ₅ H ₉ NOS	131.04049	131.19856
Histidine	H	His	C ₆ H ₇ N ₃ O	137.05891	137.14108
Phenylalanine	F	Phe	C ₉ H ₉ NO	147.06841	147.17656
Arginine	R	Arg	C ₆ H ₁₂ N ₄ O	156.10111	156.18748
Tyrosine	Y	Tyr	C ₉ H ₉ NO ₂	163.06333	163.17596
Tryptophan	W	Trp	C ₁₁ H ₁₀ N ₂ O	186.07931	186.2132

Additional Amino Acids

Name	Composition	Monoisotopic Residue Mass	Average Residue Mass
Sarcosine	C ₂ H ₅ NO	71.03711	71.0788
Homoserine lactone	C ₄ H ₅ NO	83.03711	83.0898
Homoserine	C ₄ H ₇ NO ₂	101.04768	101.10508
Pyroglutamic acid	C ₅ H ₅ NO ₂	111.03203	111.1002
Ornithine	C ₅ H ₁₀ N ₂ O	114.07931	114.1472
Carboamidomethylcysteine	C ₅ H ₈ N ₂ O ₂ S	160.03065	160.19672
Carboxymethylcysteine	C ₅ H ₇ NO ₃ S	161.01466	161.18148
Pyridylethylcysteine	C ₁₀ H ₁₂ N ₂ S	208.06703	208.28408

Nucleotides

Name	Symbol	Composition	Monoisotopic Mass	Average Mass
Ribonucleotides				
Adenosine	A	C ₁₀ H ₁₂ O ₆ N ₅ P	329.05252	329.2091
Guanosine	G	C ₁₀ H ₁₂ O ₇ N ₅ P	345.04744	345.2084
Cytidine	C	C ₉ H ₁₂ O ₇ N ₃ P	305.04129	305.1840
Uridine	U	C ₉ H ₁₁ O ₈ N ₂ P	306.02530	306.1687
Deoxyribonucleotides				
Deoxyadenosine	dA	C ₁₀ H ₁₂ O ₅ N ₅ P	313.05761	313.2097
Deoxyguanosine	dG	C ₁₀ H ₁₂ O ₆ N ₅ P	329.05252	329.2091
Deoxycytidine	dC	C ₉ H ₁₂ O ₆ N ₃ P	289.04637	289.1847
Deoxythymidine	dT	C ₁₀ H ₁₃ O ₇ N ₂ P	304.04604	304.1964

Typical Post-Translational Modifications of Proteins and Peptides

Modification	Monoisotopic Mass Change	Average Mass Change
Homoserine formed from Methionine by CNBr treatment	-29.99281	-30.0935
Pyroglutamic acid formed from Glutamine	-17.02655	-17.0306
Disulfide bond formation	-2.01565	-2.0159
C-terminal amide formed from Glycine	-0.98402	-0.9847
Deamidation of Asparagine or Glutamine	0.98402	-0.9847
Methylation	14.01565	14.0269
Oxidation of Methionine	15.99491	15.9994
Hydroxylation	15.99491	15.9994
Proteolysis of a single peptide bond	18.01060	18.0153
Formylation	27.99491	28.0104
Acetylation	42.01056	42.0373
Carboxylation of Aspartic acid or Glutamic acid	43.98983	44.0098
Carboxyamidomethylcysteine (CAM) from Cysteine	57.02146	57.0520
Carboxymethylcysteine (CME) from Cysteine	58.00548	58.0367
Sulfation	79.95682	80.0624
Phosphorylation	79.96633	79.9799
Pyridylethylcysteine (PE-Cys) from Cys	105.05785	105.1393
Cysteinylation	119.00410	119.1442
Pentoses (Ara, Rib, Xyl)	132.04226	132.1166
Deoxyhexoses (Fuc, Tha)	146.05791	146.1430
Hexosamines (GalN, GlcN)	161.06881	161.1577
Hexoses (Fru, Gal, Glc, Man)	162.05282	162.1424

Typical Post-Translational Modifications of Proteins and Peptides (continued)

Modification	Monoisotopic Mass Change	Average Mass Change
Lipoic acid (amide bond to Lysine)	188.03296	188.3147
N-acetylhexosamines (GalNAc, GlcNAc)	203.07937	203.195
Farnesylation	204.18780	204.3556
Myristoylation	210.19836	210.3598
Biotinylation (amide bond to Lysine)	226.07760	226.2994
Pyridoxal phosphate (Schiff Base formed to Lysine)	231.02966	231.1449
Palmitoylation	238.22966	238.4136
Stearoylation	266.26096	266.4674
Seranylgeranylation	272.25040	272.4741
N-acetylneuraminic acid (Sialic acid, NeuAc, NANA, SA)	291.09542	291.2579
Glutathionylation	305.06816	305.3117
N-glycolylneuraminic acid (NeuGc)	307.08003	307.2573
5'-Adenosylation	329.05252	329.2091
4'-Phosphopantetheine	339.07797	339.3294
ADP-ribosylation (from NAD)	541.06111	541.3052

Common Neutral Loss Fragments

Mass Unit	Likely Composition
1	H
15	CH ₃
17	OH
18	H ₂ O
19	F
20	HF
27	C ₂ H ₃ , HCN
28	C ₂ H ₄ , CO
30	CH ₂ O
31	CH ₃ O
32	CH ₄ O, S
33	CH ₃ + H ₂ O, HS
33	H ₂ S
35 (37)	Cl
36 (38)	HCl
42	C ₃ H ₆ , C ₂ H ₂ O, C ₂ H ₄ N
43	C ₃ H ₇ , CH ₃ CO
44	CO ₂ O, CONH ₂
45	C ₂ H ₅ O
55	C ₄ H ₇
57	C ₄ H ₉
59	C ₂ H ₃ O ₂
60	C ₂ H ₄ O ₂
64	SO ₂
79 (81)	Br
80 (82)	HBr
127	I
128	HI

Fundamental Physical Constants

	Symbol	Value
Atomic mass constant	m _u	1.66053886 x 10 ⁻²⁷ kg
Avogadro constant	N _{Av} , L	6.0221415 x 10 ²³ mol ⁻¹
Boltzmann constant	k	1.3806505 x 10 ⁻²³ J K ⁻¹
Conductance quantum	G ₀	7.748091733 x 10 ⁻⁵ S
Electric constant	ε ₀	8.854187817... x 10 ⁻¹² F m ⁻¹
Electron mass	m _e	9.1093826 x 10 ⁻³¹ kg
Electron volt	eV	1.60217653 x 10 ⁻¹⁹ J
Elementary charge	e	1.60217653 x 10 ⁻¹⁹ C
Faraday constant	F	96485.3383 C mol ⁻¹
Fine-structure constant	α	7.297352568 x 10 ⁻³
Inverse fine-structure constant	α ⁻¹	137.03599911
Magnetic constant	μ ₀	12.566370614... x 10 ⁻⁷ N A ⁻²
Magnetic flux quantum	φ ₀	2.06783372 x 10 ⁻¹⁵ Wb
Molar gas constant	R	8.314 472 J mol ⁻¹ K ⁻¹
Newtonian constant of gravitation	G	6.6742 x 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻²
Planck constant	h	6.6260693 x 10 ⁻³⁴ J s
Proton mass	m _p	1.67262171 x 10 ⁻²⁷ kg
Proton/electron mass ratio	m _p / m _e	1836.15267261
Rydberg constant	R _∞	10973731.568525 m ⁻¹
Speed of light in a vacuum	c, c ₀	299792458 m s ⁻¹
Stefan-Boltzmann constant	δ	5.670 400 x 10 ⁻⁸ W m ⁻² K ⁻⁴

