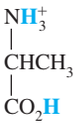
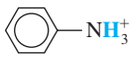
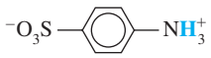
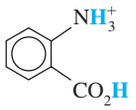
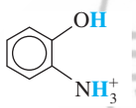
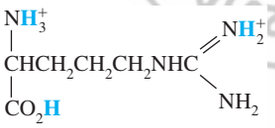
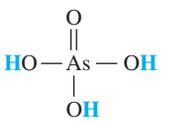
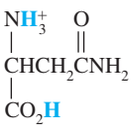
APPENDIX G Acid Dissociation Constants

Name	Structure*	Ionic strength (μ) = 0 pK_a†	Ionic strength (μ) = 0 K_a‡	μ = 0.1 M§ pK_a†
Acetic acid (ethanoic acid)	CH_3CO_2H	4.756	1.75×10^{-5}	4.56
Alanine		2.344 (CO_2H) 9.868 (NH_3)	4.53×10^{-3} 1.36×10^{-10}	2.33 9.71
Aminobenzene (aniline)		4.601	2.51×10^{-5}	4.64
4-Aminobenzenesulfonic acid (sulfanilic acid)		3.232	5.86×10^{-4}	3.01
2-Aminobenzoic acid (anthranilic acid)		2.08 (CO_2H) 4.96 (NH_3)	8.3×10^{-3} 1.10×10^{-5}	2.01 4.78
2-Aminoethanethiol (2-mercaptoethylamine)	$HSCH_2CH_2NH_3^+$	—— ——		8.21 (SH) 10.73 (NH_3)
2-Aminoethanol (ethanolamine)	$HOCH_2CH_2NH_3^+$	9.498	3.18×10^{-10}	9.52
2-Aminophenol		4.70 (NH_3) (20°) 9.97 (OH) (20°)	2.0×10^{-5} 1.05×10^{-10}	4.74 9.87
Ammonia	NH_4^+	9.245	5.69×10^{-10}	9.26
Arginine		1.823 (CO_2H) 8.991 (NH_3) —— (NH_2)	1.50×10^{-2} 1.02×10^{-9} ——	2.03 9.00 (12.1)
Arsenic acid (hydrogen arsenate)		2.24 6.96 (11.50)	5.8×10^{-3} 1.10×10^{-7} 3.2×10^{-12}	2.15 6.65 (11.18)
Arsenious acid (hydrogen arsenite)	$As(OH)_3$	9.29	5.1×10^{-10}	9.14
Asparagine		—— ——	—— ——	2.16 (CO_2H) 8.73 (NH_3)

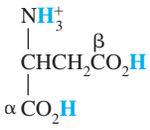
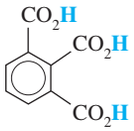
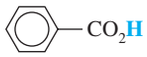
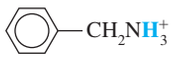
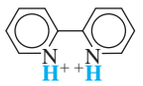
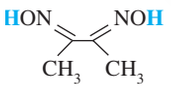
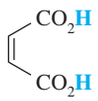
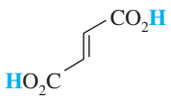
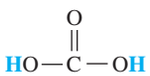
Each acid is written in its protonated form. The acidic protons are indicated in **bold type.*

†pK_a values refer to 25°C unless otherwise indicated. Values in parentheses are considered to be less reliable. Data are from A. E. Martell, R. M. Smith, and R. J. Motekaitis, NIST Database 46 (Gaithersburg, MD: National Institute of Standards and Technology, 2001).

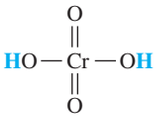
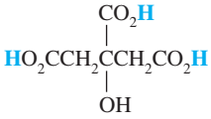
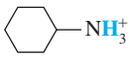
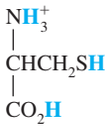
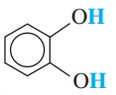
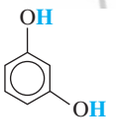
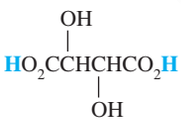
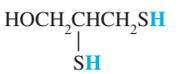
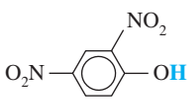
‡The accurate way to calculate K_b for the conjugate base is $pK_b = 13.995 - pK_a$ and $K_b = 10^{-pK_b}$.

§See marginal note on page 166 for distinction between pK_a at $\mu = 0$ and at $\mu = 0.1$ M.

(Continued)

Name	Structure	Ionic strength (μ) = 0 pK_a	Ionic strength (μ) = 0 K_a	μ = 0.1 M pK_a
Aspartic acid		1.990 (α-CO_2H) 3.900 (β-CO_2H) 10.002 (NH_3)	1.02×10^{-2} 1.26×10^{-4} 9.95×10^{-11}	1.95 3.71 9.96
Aziridine (dimethyleneimine)		8.04	9.1×10^{-9}	——
Benzene-1,2,3-tricarboxylic acid (hemimellitic acid)		2.86 4.30 6.28	1.38×10^{-3} 5.0×10^{-5} 5.2×10^{-7}	2.67 3.91 5.50
Benzoic acid		4.202	6.28×10^{-5}	4.01
Benzylamine		9.35	4.5×10^{-10}	9.40
2,2′-Bipyridine		—— 4.34	—— 4.6×10^{-5}	(1.3) 4.41
Boric acid (hydrogen borate)	$B(OH)_3$	9.237 (12.74) (20°) (13.80) (20°)	5.79×10^{-10} 1.82×10^{-13} 1.58×10^{-14}	8.98 —— ——
Bromoacetic acid	$BrCH_2CO_2H$	2.902	1.25×10^{-3}	2.71
Butane-2,3-dione dioxime (dimethylglyoxime)		10.66 (12.0)	2.2×10^{-11} 1×10^{-12}	10.45 (11.9)
Butanoic acid	$CH_3CH_2CH_2CO_2H$	4.818	1.52×10^{-5}	4.62
cis-Butenedioic acid (maleic acid)		1.92 6.27	1.20×10^{-2} 5.37×10^{-7}	1.75 5.84
trans-Butenedioic acid (fumaric acid)		3.02 4.48	9.5×10^{-4} 3.3×10^{-5}	2.84 4.09
Butylamine	$CH_3CH_2CH_2CH_2NH_3^+$	10.640	2.29×10^{-11}	10.66
Carbonic acid* (hydrogen carbonate)		6.351 10.329	4.46×10^{-7} 4.69×10^{-11}	6.13 9.91
Chloroacetic acid	$ClCH_2CO_2H$	2.865	1.36×10^{-3}	2.69
3-Chloropropanoic acid	$ClCH_2CH_2CO_2H$	4.11	7.8×10^{-5}	3.92
Chlorous acid (hydrogen chlorite)	HOCl=O	1.96	1.10×10^{-2}	——

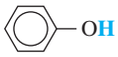
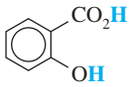
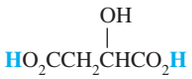
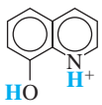
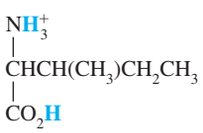
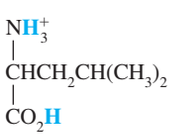
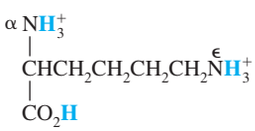
**The concentration of "carbonic acid" is considered to be the sum $[H_2CO_3] + [CO_2(aq)]$. See Box 6-4.*

Name	Structure	Ionic strength (μ) = 0 pK_a	Ionic strength (μ) = 0 K_a	μ = 0.1 M pK_a
Chromic acid (hydrogen chromate)		(−0.2) (20°) 6.51	1.6 3.1×10^{-7}	(−0.6) (20°C) 6.05
Citric acid (2-hydroxypropane-1,2,3-tricarboxylic acid)		3.128 4.761 6.396	7.44×10^{-4} 1.73×10^{-5} 4.02×10^{-7}	2.90 4.35 5.70
Cyanoacetic acid	$NCCH_2CO_2H$	2.472	3.37×10^{-3}	——
Cyclohexylamine		10.567	2.71×10^{-11}	10.62
Cysteine		(1.7) (CO_2H) 8.36 (SH) 10.74 (NH_3)	2×10^{-2} 4.4×10^{-9} 1.82×10^{-11}	(1.90) 8.18 10.30
Dichloroacetic acid	Cl_2CHCO_2H	(1.1)	8×10^{-2}	(0.9)
Diethylamine	$(CH_3CH_2)_2NH_2^+$	11.00	1.0×10^{-11}	11.04
1,2-Dihydroxybenzene (catechol)		9.45 ——	3.5×10^{-10} ——	9.26 (13.3)
1,3-Dihydroxybenzene (resorcinol)		—— ——	—— ——	9.30 11.06
D-2,3-Dihydroxybutanedioic acid (D-tartaric acid)		3.036 4.366	9.20×10^{-4} 4.31×10^{-5}	2.82 3.97
2,3-Dimercaptopropanol		—— ——	—— ——	8.63 10.65
Dimethylamine	$(CH_3)_2NH_2^+$	10.774	1.68×10^{-11}	10.81
2,4-Dinitrophenol		4.114	7.69×10^{-5}	3.92
Ethane-1,2-dithiol	$HSCH_2CH_2SH$	—— ——	—— ——	8.85 (30°C) 10.43 (30°C)
Ethylamine	$CH_3CH_2NH_3^+$	10.673	2.12×10^{-11}	10.69
Ethylenediamine (1,2-diaminoethane)	$H_3\overset{+}{N}CH_2CH_2\overset{+}{N}H_3$	6.848 9.928	1.42×10^{-7} 1.18×10^{-10}	7.11 9.92

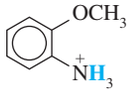
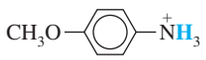
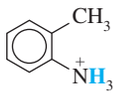
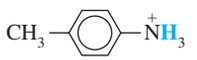
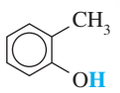
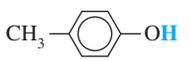
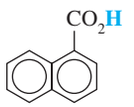
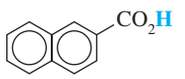
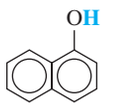
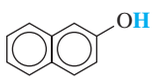
(Continued)

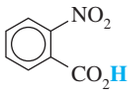
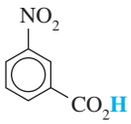
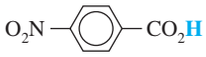
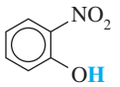
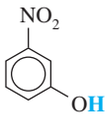
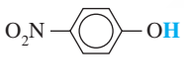
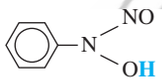
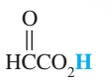
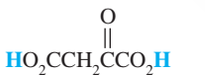
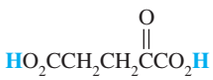
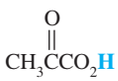
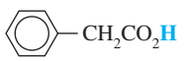
Name	Structure	Ionic strength (μ) = 0 pK_a	Ionic strength (μ) = 0 K_a	μ = 0.1 M pK_a
Ethylenedinitrilotetraacetic acid (EDTA)	$(HO_2CCH_2)_2\overset{+}{N}HCH_2CH_2\overset{+}{N}H(CH_2CO_2H)_2$	—— (CO_2H) —— (CO_2H) —— (CO_2H) —— (CO_2H) 6.273 (NH) 10.948 (NH)	—— —— —— —— 5.3×10^{-7} 1.13×10^{-11}	(0.0) (CO_2H) (μ = 1 M) (1.5) (CO_2H) 2.00 (CO_2H) 2.69 (CO_2H) 6.13 (NH) 10.37 (NH)
Formic acid (methanoic acid)	HCO_2H	3.744	1.80×10^{-4}	3.57
Glutamic acid	NH_3^+ $CHCH_2CH_2\overset{\gamma}{C}O_2H$ $\alpha\ CO_2H$	2.160 (α-CO_2H) 4.30 (γ-CO_2H) 9.96 (NH_3)	6.92×10^{-3} 5.0×10^{-5} 1.10×10^{-10}	2.16 4.15 9.58
Glutamine	NH_3^+ O $CHCH_2CH_2CNH_2$ CO_2H	—— ——	—— ——	2.19 (CO_2H) 9.00 (NH_3)
Glycine (aminoacetic acid)	NH_3^+ CH_2 CO_2H	2.350 (CO_2H) 9.778 (NH_3)	4.47×10^{-3} 1.67×10^{-10}	2.33 9.57
Guanidine	$^+NH_2$ $H_2N-C-NH_2$	——	——	(13.5) (μ = 1 M)
1,6-Hexanedioic acid (adipic acid)	$HO_2CCH_2CH_2CH_2CH_2CO_2H$	4.424 5.420	3.77×10^{-5} 3.80×10^{-6}	4.26 5.04
Hexane-2,4-dione	O O $CH_3CCH_2CCH_2CH_3$	9.38	4.2×10^{-10}	9.11 (20°C)
Histidine	NH_3^+ $CHCH_2$ — NH, $\overset{+}{N}H$ CO_2H	(1.6) (CO_2H) 5.97 (NH) 9.28 (NH_3)	3×10^{-2} 1.07×10^{-6} 5.2×10^{-10}	(1.7) 6.05 9.10
Hydrazine	$H_3\overset{+}{N}-\overset{+}{N}H_3$	−0.99 7.98	1.0×10^{1} 1.05×10^{-8}	(−0.21) (μ = 0.5 M) 8.07
Hydrazoic acid (hydrogen azide)	$HN=\overset{+}{N}=\overset{-}{N}$	4.65	2.2×10^{-5}	4.45
Hydrogen cyanate	HOC≡N	3.48	3.3×10^{-4}	——
Hydrogen cyanide	HC≡N	9.21	6.2×10^{-10}	9.04
Hydrogen fluoride	HF	3.17	6.8×10^{-4}	2.94
Hydrogen peroxide	HOOH	11.65	2.2×10^{-12}	——
Hydrogen sulfide	H_2S	7.02 14.0*	9.5×10^{-8} $1.0 \times 10^{-14*}$	6.82 ——
Hydrogen thiocyanate	HSC≡N	(−1.1) (20°C)	1.3×10^{1}	——
Hydroxyacetic acid (glycolic acid)	$HOCH_2CO_2H$	3.832	1.48×10^{-4}	3.62

D. J. Phillips and S. L. Phillips. "High Temperature Dissociation Constants of HS^- and the Standard Thermodynamic Values for S^{2-}," J. Chem. Eng. Data **2000, 45, 981.*

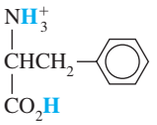
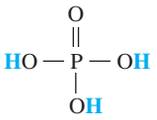
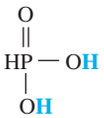
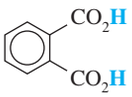
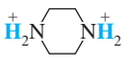
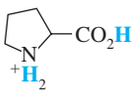
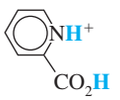
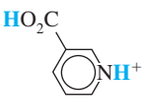
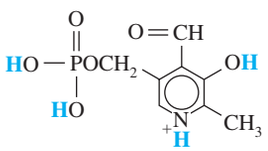
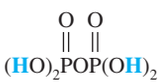
Name	Structure	Ionic strength (μ) = 0 pK_a	Ionic strength (μ) = 0 K_a	μ = 0.1 M pK_a
Hydroxybenzene (phenol)		9.997	1.01×10^{-10}	9.78
2-Hydroxybenzoic acid (salicylic acid)		2.972 (CO_2H) (13.7) (OH)	1.07×10^{-3} 2×10^{-14}	2.80 (13.4)
L-Hydroxybutanedioic acid (malic acid)		3.459 5.097	3.48×10^{-4} 8.00×10^{-6}	3.24 4.68
Hydroxylamine		5.96 (NH) (13.74) (OH)	1.10×10^{-6} 1.8×10^{-14}	5.96 ——
8-Hydroxyquinoline (oxine)		4.94 (NH) 9.82 (OH)	1.15×10^{-5} 1.51×10^{-10}	4.97 9.65
Hypobromous acid (hydrogen hypobromite)	HOBr	8.63	2.3×10^{-9}	——
Hypochlorous acid (hydrogen hypochlorite)	HOCl	7.53	3.0×10^{-8}	——
Hypoiodous acid (hydrogen hypoiodite)	HOI	10.64	2.3×10^{-11}	——
Hypophosphorous acid (hydrogen hypophosphite)		(1.3)	5×10^{-2}	(1.1)
Imidazole (1,3-diazole)		6.993 (14.5)	1.02×10^{-7} 3×10^{-15}	7.00 ——
Iminodiacetic acid		(1.85) (CO_2H) 2.84 (CO_2H) 9.79 (NH_2)	1.41×10^{-2} 1.45×10^{-3} 1.62×10^{-10}	(1.77) 2.62 9.34
Iodic acid (hydrogen iodate)		0.77	0.17	——
Iodoacetic acid	ICH_2CO_2H	3.175	6.68×10^{-4}	2.98
Isoleucine		2.318 (CO_2H) 9.758 (NH_3)	4.81×10^{-3} 1.75×10^{-10}	2.26 9.60
Leucine		2.328 (CO_2H) 9.744 (NH_3)	4.70×10^{-3} 1.80×10^{-10}	2.32 9.58
Lysine		(1.77) (CO_2H) 9.07 (α-NH_3) 10.82 (ϵ-NH_3)	1.7×10^{-2} 8.5×10^{-10} 1.51×10^{-11}	2.15 9.15 10.66

(Continued)

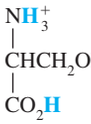
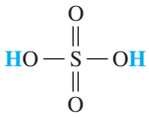
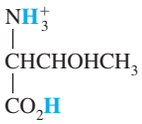
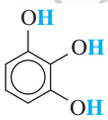
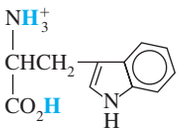
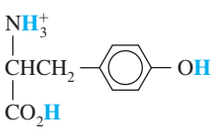
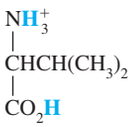
Name	Structure	Ionic strength (μ) = 0		μ = 0.1 M
		pK_a	K_a	pK_a
Malonic acid (propanedioic acid)	$HO_2CCH_2CO_2H$	2.847 5.696	1.42×10^{-3} 2.01×10^{-6}	2.65 5.27
Mercaptoacetic acid (thioglycolic acid)	$HSCH_2CO_2H$	3.64 (CO_2H) 10.61 (SH)	2.3×10^{-4} 2.5×10^{-11}	3.48 10.11
2-Mercaptoethanol	$HSCH_2CH_2OH$	9.72	1.9×10^{-10}	9.40
Methionine	$CH_3SCH_2CH_2CH(NH_3^+)CO_2H$	—— ——	—— ——	2.18 (CO_2H) 9.08 (NH_3)
2-Methoxyaniline (*o*-anisidine)		4.526	2.98×10^{-5}	——
4-Methoxyaniline (*p*-anisidine)		5.357	4.40×10^{-6}	5.33
Methylamine	$CH_3NH_3^+$	10.632	2.33×10^{-11}	10.65
2-Methylaniline (*o*-toluidine)		4.447	3.57×10^{-5}	——
4-Methylaniline (*p*-toluidine)		5.080	8.32×10^{-6}	5.09
2-Methylphenol (*o*-cresol)		10.31	4.9×10^{-11}	10.09
4-Methylphenol (*p*-cresol)		10.269	5.5×10^{-11}	10.04
Morpholine (perhydro-1,4-oxazine)		8.492	3.22×10^{-9}	——
1-Naphthoic acid		3.67	2.1×10^{-4}	——
2-Naphthoic acid		4.16	6.9×10^{-5}	——
1-Naphthol		9.416	3.84×10^{-10}	9.14
2-Naphthol		9.573	2.67×10^{-10}	9.31
Nitrilotriacetic acid	$HN^+(CH_2CO_2H)_3$	—— (CO_2H) 2.0 (CO_2H) (25°) 2.940 (CO_2H) (20°) 10.334 (NH) (20°)	—— 0.010 1.15×10^{-3} 4.63×10^{-11}	(1.0) 1.81 2.52 9.46

Name	Structure	Ionic strength (μ) = 0		μ = 0.1 M
		pK_a	K_a	pK_a
2-Nitrobenzoic acid		2.185	6.53×10^{-3}	——
3-Nitrobenzoic acid		3.449	3.56×10^{-4}	3.28
4-Nitrobenzoic acid		3.442	3.61×10^{-4}	3.28
Nitroethane	$CH_3CH_2NO_2$	8.57	2.7×10^{-9}	——
2-Nitrophenol		7.230	5.89×10^{-8}	7.04
3-Nitrophenol		8.37	4.3×10^{-9}	8.16
4-Nitrophenol		7.149	7.10×10^{-8}	6.96
N-Nitrosophenylhydroxylamine (cupferron)		——	——	4.16
Nitrous acid	HON=O	3.15	7.1×10^{-4}	——
Oxalic acid (ethanedioic acid)	HO_2CCO_2H	1.250 4.266	5.62×10^{-2} 5.42×10^{-5}	(1.2) 3.80
Oxoacetic acid (glyoxylic acid)		3.46	3.5×10^{-4}	3.05
Oxobutanedioic acid (oxaloacetic acid)		2.56 4.37	2.8×10^{-3} 4.3×10^{-5}	2.26 3.90
2-Oxopentanedioic (α-ketoglutaric acid)		—— ——	—— ——	(1.9) (μ = 0.5 M) 4.44 (μ = 0.5 M)
2-Oxopropanoic acid (pyruvic acid)		2.48	3.3×10^{-3}	2.26
1,5-Pentanedioic acid (glutaric acid)	$HO_2CCH_2CH_2CH_2CO_2H$	4.345 5.422	4.52×10^{-5} 3.78×10^{-6}	4.19 5.06
Pentanoic acid (valeric acid)	$CH_3CH_2CH_2CH_2CO_2H$	4.843	1.44×10^{-5}	4.63 (18°C)
1,10-Phenanthroline		—— 4.91	—— 1.23×10^{-5}	(1.8) 4.92
Phenylacetic acid		4.310	4.90×10^{-5}	4.11

(Continued)

Name	Structure	Ionic strength (μ) = 0 pK_a	Ionic strength (μ) = 0 K_a	μ = 0.1 M pK_a
Phenylalanine		2.20 (CO_2H) 9.31 (NH_3)	6.3×10^{-3} 4.9×10^{-10}	2.18 9.09
Phosphoric acid* (hydrogen phosphate)		2.148 7.198 12.375	7.11×10^{-3} 6.34×10^{-8} 4.22×10^{-13}	1.92 6.71 11.52
Phosphorous acid (hydrogen phosphite)		(1.5) 6.78	3×10^{-2} 1.66×10^{-7}	—— ——
Phthalic acid (benzene-1,2-dicarboxylic acid)		2.950 5.408	1.12×10^{-3} 3.90×10^{-6}	2.76 4.92
Piperazine (perhydro-1,4-diazine)		5.333 9.731	4.65×10^{-6} 1.86×10^{-10}	5.64 9.74
Piperidine		11.125	7.50×10^{-12}	11.08
Proline		1.952 (CO_2H) 10.640 (NH_2)	1.12×10^{-2} 2.29×10^{-11}	1.89 10.46
Propanoic acid	$CH_3CH_2CO_2H$	4.874	1.34×10^{-5}	4.69
Propenoic acid (acrylic acid)	$H_2C{=}CHCO_2H$	4.258	5.52×10^{-5}	——
Propylamine	$CH_3CH_2CH_2NH_3^+$	10.566	2.72×10^{-11}	10.64
Pyridine (azine)		5.20	6.3×10^{-6}	5.24
Pyridine-2-carboxylic acid (picolinic acid)		(1.01) (CO_2H) 5.39 (NH)	9.8×10^{-2} 4.1×10^{-6}	(0.95) 5.21
Pyridine-3-carboxylic acid (nicotinic acid)		2.03 (CO_2H) 4.82 (NH)	9.3×10^{-3} 1.51×10^{-5}	2.08 4.69
Pyridoxal-5-phosphate		—— —— —— ——	—— —— —— ——	(1.4) (POH) 3.51 (OH) 6.04 (POH) 8.25 (NH)
Pyrophosphoric acid (hydrogen diphosphate)		(0.9) 2.28 6.70 9.40	0.13 5.2×10^{-3} 2.0×10^{-7} 4.0×10^{-10}	(0.8) (1.9) 5.94 8.25

*pK_3 from A. G. Miller and J. W. Macklin, Anal. Chem. **1983,** 55, 684.

Name	Structure	Ionic strength (μ) = 0		μ = 0.1 M
		pK_a	K_a	pK_a
Pyrrolidine		11.305	4.95×10^{-12}	11.3
Serine		2.187 (CO_2H) 9.209 (NH_3)	6.50×10^{-3} 6.18×10^{-10}	2.16 9.05
Succinic acid (butanedioic acid)		4.207 5.636	6.21×10^{-5} 2.31×10^{-6}	3.99 5.24
Sulfuric acid (hydrogen sulfate)		1.987 (pK_2)	1.03×10^{-2}	1.54
Sulfurous acid (hydrogen sulfite)		1.857 7.172	1.39×10^{-2} 6.73×10^{-8}	1.66 6.85
Thiosulfuric acid (hydrogen thiosulfate)		(0.6) (1.6)	0.3 0.03	—— (1.3)
Threonine		2.088 (CO_2H) 9.100 (NH_3)	8.17×10^{-3} 7.94×10^{-10}	2.20 8.94
Trichloroacetic acid	Cl_3CCO_2H	(−0.5)	3	——
Triethanolamine	$(HOCH_2CH_2)_3NH^+$	7.762	1.73×10^{-8}	7.85
Triethylamine	$(CH_3CH_2)_3NH^+$	10.72	1.9×10^{-11}	10.76
1,2,3-Trihydroxybenzene (pyrogallol)		—— —— ——	—— —— ——	8.96 11.00 (14.0) (20°C)
Trimethylamine	$(CH_3)_3NH^+$	9.799	1.59×10^{-10}	9.82
Tris(hydroxymethyl)amino-methane (tris or tham)	$(HOCH_2)_3CNH_3^+$	8.072	8.47×10^{-9}	8.10
Tryptophan		—— ——	—— ——	2.37 (CO_2H) 9.33 (NH_3)
Tyrosine		—— —— ——	—— —— ——	2.41 (CO_2H) 8.67 (NH_3) 11.01 (OH)
Valine		2.286 (CO_2H) 9.719 (NH_3)	5.18×10^{-3} 1.91×10^{-10}	2.27 9.52
Water*	H_2O	13.997	1.01×10^{-14}	——

**The constant given for water is K_w.*