Zwitterion behavior of an amino acid. (... continuation of amino.mcd)
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Assign an index number and the pK values (dissociation constants) to each of the 20 amino acids. We deliberately assign an out-of-bound index number (e.g., 999) to those amino acids whose data are missing. This way, Mathcad will flag invalid results. As dissociation data become available, we can restore a proper index number. (We use tryptophan to demonstrate this, although we really have data for tryptophan.) Source of dissociation data: Dawson, Elliott, Elliotee, and Jones, "Data for Biochemical Research," 3rd Ed., Oxford Science Publications, 1986. The data was reproduced in Voet & Voet, "Biochemistry," 2nd Ed., Wiley, 1995.

Amino Acid (full name)		Amino Acid (3-letter)		pK_1 (-COOH)	pK_2 (-NH$_2$)	pK_R (-R group)
Alanine	0	Ala	0	2.35	9.87	0
Arginine	1	Arg	1	1.82	8.99	12.48
Asparagine	2	Asn	2	2.14	8.72	0
AsparticAcid	3	Asp	3	1.99	9.90	3.90
Cysteine	4	Cys	4	1.92	10.70	8.37
GlutamicAcid	5	Glu	5	2.19	9.67	4.07
Glutamine	6	Gln	6	2.10	9.47	0
Glycine	7	Gly	7	2.35	9.78	0
Histidine	8	His	8	1.80	9.33	6.04
Isoleucine	9	Ile	9	2.32	9.76	0
Leucine	10	Leu	10	2.33	9.74	0
Lysine	11	Lys	11	2.16	9.06	10.54
Methionine	12	Met	12	2.13	9.28	0
Phenylalanine	13	Phe	13	2.20	9.31	0
Proline	14	Pro	14	1.95	10.64	0
Serine	15	Ser	15	2.19	9.21	0
Threonine	16	Thr	16	2.09	9.10	0
Tryptophan	999	Trp	999	2.46	9.41	0
Tyrosine	18	Tyr	18	2.20	9.21	10.46
Valine	19	Val	19	2.29	9.74	0

The vectors are defined as (index) := , (3-letter) := , pK_1 := , pK_2 := , pK_R := for the columns above.

The fraction of amino acid in cation, neutral, and anion are given below (from amino.mcd).

$$A_{cation}\left(pH, pK_1, pK_2\right) := \frac{10^{-2 \cdot pH}}{10^{-2 \cdot pH} + 10^{-pK_1 - pH} + 10^{-pK_1 - pK_2}}$$

$$A_{neutral}\left(pH, pK_1, pK_2\right) := \frac{10^{-pK_1 - pH}}{10^{-2 \cdot pH} + 10^{-pK_1 - pH} + 10^{-pK_1 - pK_2}}$$

$$A_{anion}\left(pH, pK_1, pK_2\right) := \frac{10^{-pK_1 - pK_2}}{10^{-2 \cdot pH} + 10^{-pK_1 - pH} + 10^{-pK_1 - pK_2}}$$

Re-define the above fractions /w the name of a specific amino acid as a function argument.

$$f_{cation}(pH, AA) := \frac{10^{-2 \cdot pH}}{10^{-2 \cdot pH} + 10^{-pK_{1AA} - pH} + 10^{-pK_{1AA} - pK_{2AA}}}$$

$$f_{neutral}(pH, AA) := \frac{10^{-pK_{1AA} - pH}}{10^{-2 \cdot pH} + 10^{-pK_{1AA} - pH} + 10^{-pK_{1AA} - pK_{2AA}}}$$

$$f_{anion}(pH, AA) := \frac{10^{-pK_{1AA} - pK_{2AA}}}{10^{-2 \cdot pH} + 10^{-pK_{1AA} - pH} + 10^{-pK_{1AA} - pK_{2AA}}}$$

Example: Alanine at $pH := 7$

$f_{cation}(pH, Alanine) = 2.236 \cdot 10^{-5}$ $f_{cation}(pH, Ala) = 2.236 \cdot 10^{-5}$

$f_{neutral}(pH, Alanine) = 0.999$ $f_{neutral}(pH, Ala) = 0.999$

$f_{anion}(pH, Alanine) = 0.001$ $f_{anion}(pH, Ala) = 0.001$

We can use either full name or 3-letter abbreviation as the argument.

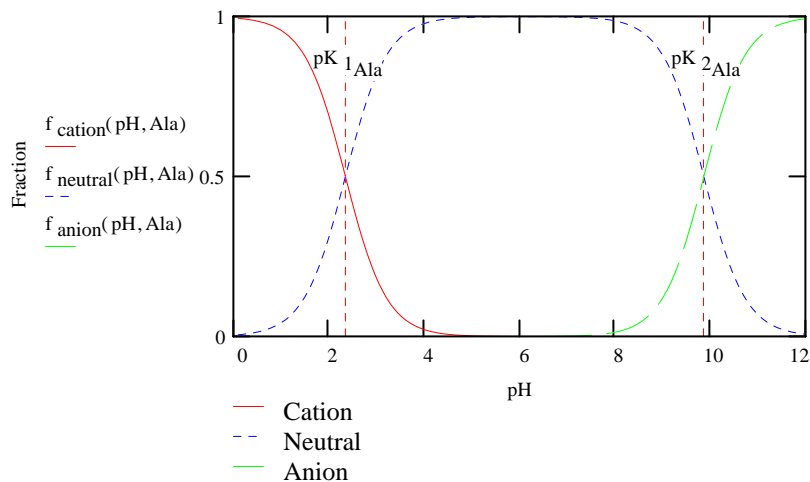However, Mathcad flags an error message when pK data are missing.

$f_{anion}(pH, Tryptophan) =$ $f_{neutral}(pH, Tryptophan) =$ $f_{cation}(pH, Tryptophan) =$

index out of bounds   index out of bounds   index out of bounds

Plot of alanine's pH dependence for a range of pH values: $pH := 0.1, 0.2 .. 12$

Compare the zwitterions of different amino acid species.

$f_{neutral}(pH, Ala)$

$f_{neutral}(pH, His)$

$f_{neutral}(pH, Thr)$

$f_{neutral}(pH, Cys)$

Alanine
Histidine
Threonine
Cysteine