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**THERMODYNAMIC DATA BASE FOR THE AQUATIC
CHEMICAL SPECIATION SOFTWARE PACKAGE:
MACS80 (Version 5/1990-VAX and MS-DOS[®]).**

3rd edition

by

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ABSTRACT

Wagemann, R. 1994. Compilation of the Thermodynamic data used by the Chemical Speciation Software Package: MACS80 (Version 5/1990-VAX and MS-DOS[®]) 3rd edition. Can. Tech. Rep. Aquat. Sci. 1991: iv+113 p.

The report is a compilation of the thermodynamic data base used by the MACS80 chemical speciation computer program together with the defining chemical equations and the chemical species considered by the program. Also presented are some comparative data between this and thirteen other chemical speciation programs as a way of verifying the algorithm used by MACS80, as well as some error estimates of the calculated species concentrations using the Monte Carlo approach. A number of equations are presented which the program uses and pertinent explanations of their function are given.

Key words: thermodynamic data base; metals; chemical speciation, algorithms; fresh water; equilibrium constants; compilation.

RÉSUMÉ

Wagemann, R. 1994. Compilation des données thermodynamiques utilisées par le progiciel de caractérisation chimique MACS80 (Version 5/1990-VAX and MS-DOS[®]), 3^e édition. Can. Tech. Rep. Aquat. Sci. 1991: iv+113 p.

Le rapport est une compilation des données thermodynamiques utilisées par le progiciel de caractérisation chimique MACS80, ainsi que des équations chimiques servant aux définitions et des espèces chimiques considérées dans le progiciel. On présente aussi certaines données comparatives tirées de ce progiciel et de treize autres progiciels de caractérisation chimique, dans le but de vérifier l'algorithme utilisé par le MACS80, ainsi que certaines estimations des erreurs sur les concentrations calculées des espèces obtenues à l'aide de la méthode de Monte Carlo. On présente un certain nombre d'équations utilisées par le progiciel et on donne des explications pertinentes de leur fonction.

Mots clés: thermodynamique compilation; metaux; détermination d'espèces chimiques; algorithmes; eau douce; d'équilibre chimique; compilation.

INTRODUCTION

This report is a compilation of the thermodynamic data used in the MACS80 Chemical speciation computer program and is a companion to the two previously published reports on this program, namely the source code (Wagemann et al. 1990) and the User's Guide (Wagemann and Regehr, 1992).

EQUILIBRIUM CONSTANTS

Over 300 equilibrium constants used by the MACS80 Chemical Speciation computer program to calculate the concentration of chemical species in a freshwater system are given in Appendix 1 together with the corresponding chemical equations used to define these constants. The expressions for the equilibrium constants are written in the standard fashion with the right-hand side components of the chemical equation in the numerator and the left-hand side components in the denominator. The equivalent exponential pH expression below, is used instead of the hydrogen ion activity wherever hydrogen ion activity occurs in an equation.

The literature sources for the constants were carefully selected. Many constants were taken from Smith and Martell's (1976) "Critical Stability Constants", Vol. 4. Sources for constants are listed under "References for Appendices" at the end of this report.

$$[H^+] = 10^{-pH}$$

Only infrequently is logK also tabulated in Appendix 1, as this quantity is easily calculated by the user from the given K

values i.e. equilibrium constants.

The species are calculated as activities by the computer program but the final results can be obtained in terms of various concentration units converted from activities by utilization of the calculated activity coefficients (γ). Activity coefficients are calculated by the program using the extended Debye-Hückel equation (valid in the range $0 < I \leq 0.2$). "A" and "B" are constants that depend on temperature, " z_i " is the charge on the

$$-\log_{10} \gamma_i = \frac{A \times z_i^2 \times \sqrt{I}}{1 + B \times \bar{a}_i \times \sqrt{I}}$$

ion, " \bar{a}_i " is the approximate radius of the ion and "I" is the ionic strength of the solution in units of molality as defined below:

$$I = \frac{1}{2} \sum m_i \times z_i^2$$

In the above equation " m_i " is the molality of the ion and " z_i ", the charge on the ion. "A" and "B" were expressed as a function of temperature as follows:

$$A = 0.4875 \times e^{1.783 \times 10^{-3} \times t}$$

$$B = 0.3239 \times e^{5.933 \times 10^{-4} \times t}$$

The numerical coefficients in the above two equations were obtained by regression of published numerical data of "A" and "B" as a function of temperature (Garrels and Christ, 1965; Manov et al. 1943). If the ionic strength is not given, it is calculated by the program using the following relationship:

$$I = S \times 1.8 \times 10^{-5}$$

"S" (mSiemens/cm), is the conductivity of the freshwater in question. The above equation was determined from published conductivity and ionic strength data (Ponnamperuma, 1966), for fresh water supplemented by similar data (produced in our laboratory) for Lake Winnipeg.

For convenience and economy the combination of activity coefficients occurring in each equation is defined in column 1 of Appendix 1, by the single symbol " α_i ". The subscript index is the same as that on the corresponding K's.

TEMPERATURE DEPENDENCE OF K's

The chemical species concentrations are calculated by the MACS80 program using the equilibrium approach. In the computer program the values of K are calculated from the following equation:

$$K_t = e^{C + \frac{m}{273.15 + t}}$$

and the appropriate "C" and "m" values are stored as a data base rather than the K values themselves. Both "C" and "m" depend on the standard enthalpy change for the reaction, ΔH_r° (calories/mole). When the latter quantity is zero, then $K_t = K_{25}$, i.e. the equilibrium constant at 25° C. "m" and "C" are defined as follows:

$$m = -0.5032 \times \Delta H_r^\circ$$

$$C = 1.69 \times 10^{-3} \times \Delta H_r^\circ + 2.302 \times \log_{10}(K_{25})$$

Where the enthalpy was not available for a

reaction, m=0 in Appendix 3. Calculations are performed for a specified temperature only for those reactions for which m ≠ 0. For reactions for which m=0, the speciation calculations are performed at 25° C (i.e. K_{25}) irrespective of the specified temperature.

CHEMICAL SPECIES

The kind of species for which concentrations can be calculated by the program are listed in Appendix 2, together with their ionic charges and radii and a coding symbol (χ_i) in column 2 for each ion, which simply identifies each ion more economically than a chemical formula. The numerical subscript on the symbol codes the species. Although the calculation units of the program are M, the program can provide hard-copy results in six different concentration units chosen by the user, namely mg/L, log(mg/L), M, log(M), %mg/L, and %M. To avoid ambiguity, metric concentrations are expressed in terms of one of the elements making up the species e.g. mg C/L for CO_3^{\pm} rather than mg $\text{CO}_3^{\pm}/\text{L}$.

The appropriate formula weights (conversion factors) to convert from molar to metric concentration units used by the program are also listed in Appendix 2. Molar concentration i.e. molarity (M) [the number of gram-molecular-weights (or gram-ionic-weights) of a solute (or ionic species) in a liter of solution] and molal concentration i.e. molality (m) [the number of gram-molecular-weights (or gram-ionic-weights) of a solute (or ionic species) in 1000 g of water] are not differentiated here because they differ insignificantly at such low concentrations of species as are found in fresh waters.

The α_i 's are defined in Appendix 3, and indexed (i) in terms of chemical equations. The γ_i 's are defined in Appendix 2, and indexed (i) in terms of chemical species.

VERIFICATION OF THE ALGORITHM

In a comparative study, Nordstrom et al. 1979, published input test data (river water composition) and the calculated results based on these data by 13 different chemical speciation computer programs. Using these test data, calculations were also performed with the MACS80 chemical speciation program and the output for a representative sample of species was compared to results obtained by the other programs, Table 1. At 9.5° C, it was possible to compare MACS80 results to those of 10 other programs: EQUIL, EQ3, IONPAIR, MIRE, MINEQL, REDEQL2, SOLMNEQ, WATEQF, WATEQ2, WATSPEC. At 25° C, results could be compared to values by one other program namely, MINEQL2. Other programs either did not calculate at this temperature, or imposed incomparable conditions (equilibration with solid mineral phases) not stipulated in the test and not imposed by other participants. The results obtained by the MACS80 program are very comparable, at both temperatures, to those obtained by the other programs.

ERROR ESTIMATES

The estimation of errors in the calculated species concentrations arising from errors in the equilibrium constants was investigated. Error propagation formulas could not be applied to this problem because of the relatively large number of equilibrium constants involved and their varied

combination (multiplication, division) in the coefficients of the polynomial functions of each species. To estimate the errors, the Monte Carlo reiterative approach was used on a representative sample of species. A $\pm 10\%$ error was assigned to each equilibrium constant. The sign of the error was changed randomly for each constant after each iteration. Three hundred such reiterations were performed initially, but 30 were found to be sufficient to produce the same results as 300 reiterations. After each iteration, the calculated concentration of each species was obviously somewhat different due to the change in sign of some of the error terms associated with each equilibrium constant involved in the calculation of that species. After a sufficient number of reiterations the mean and standard deviations of the species concentrations were calculated and used to determine the coefficients of variation, Table 2. The calculated errors were normally distributed (Chi-square, $P \geq 0.98$). The errors (Table 2) are different for different chemical species because the number of equilibrium constants involved in the calculation of each species is not the same and their combination (division, multiplication) in the coefficients of each polynomial equation for the different species is also not the same. Clearly, this had a significant influence on the magnitude of the error.

The pH also influenced the size of the errors. The different species were influenced differently by this variable but most frequently, the errors increased with increasing pH.

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Table 1. Comparison of species concentrations calculated with the MACS80 program and other programs at 25° C and 9° C.

Species	-logM			
	Other Programs ¹ 25° C	MACS80 25° C	Other Programs ² 9.5° C	MACS80 9.5° C
CO ₃ ⁼	5.01	5.169	5.346 - 5.11	5.348
HCO ₃ ⁻	2.93	2.923	2.93 - 2.91	2.924
Ca ⁺⁺	---	3.528	3.539 - 3.522	3.526
Mg ⁺⁺	3.53	3.520	3.54 - 3.518	3.519
SO ₄ ⁼	4.14	4.127	4.164 - 4.12	4.127
CaCO ₃ ⁰	---	5.732	6.001 - 5.27	5.904
CaSO ₄ ⁰	---	5.538	5.58 - 5.533	5.531
MgCO ₃ ⁰	5.55	5.991	6.157 - 5.470	6.164
MgSO ₄ ⁰	5.47	5.579	5.767 - 5.45	5.573
CaHCO ₃ ⁺	---	5.542	5.723 - 5.27	5.694
MgHCO ₃ ⁺	5.16	5.610	6.027 - 5.21	5.738
Cl ⁻	3.55	3.554	3.558 - 3.401	3.554
Cu ⁺⁺	9.67	10.420	14.772 - 8.763	10.405
Cu(OH) ₂ ⁰	13.68	8.172	13.22 - 9.045	8.154
Cd ⁺⁺	9.10	9.726	11.612 - 9.41	9.702
CdOH ⁺	10.15	11.887	12.651 - 11.46	11.861
H ₂ PO ₄ ⁻	---	6.694	6.694 - 6.622	6.640
HPO ₄ ⁼	---	5.813	5.818 - 5.773	5.821
H ₂ S	---	8.273	8.403 - 8.071	8.068
HS ⁻	---	7.279	7.544 - 7.268	7.306
S ⁼	---	13.100	17.140 - 12.613	13.423
PO ₄ ⁼	---	10.032	10.189 - 10.03	10.044
Fe ²⁺	---	6.588	12.167 - 6.579	6.580
FeOH ⁺	---	8.144	26.711 - 6.855	8.667
CdHS ⁺	---	9.516	9.078	9.516
Hg ⁺²	21.07	33.341	41.872 - 16.875	33.290

¹ includes MINEQL2 program

² includes EQUIL, EQ3, IONPAIR, WATEQF, WATEQ2, WATSPEC, MIRE, REDEQL2, SOLMNEQ, MINEQL/REDEQL2 programs

³ --- data calculated under conditions not stipulated by test criteria and therefore not suitable for comparison here, or data are not available.

TABLE 2. Error estimates by the Monte Carlo reiterative procedure in the concentration of some chemical species arising from a random $\pm 10\%$ error in the equilibrium constants.

Species	Species Index No.	$\pm \%$ Coefficient of Variation -----		
		pH 8.0	pH 7.2	pH 6.0
$\text{CO}_3^=$	χ_1	4.3	4.2	3.8
HCO_3^-	χ_2	0.09	0.4	2.4
Cu^{++}	χ_{18}	2.9	2.5	0.46
CuCO_3	χ_{19}	5.6	3.8	5.0
Cu(OH)_2^0	χ_{22}	0.81	2.7	3.3
CuA_2	χ_{30}	4.7	4.1	3.1
Cd^{++}	χ_{40}	1.4	1.6	0.58
CdCl^+	χ_{47}	3.9	3.8	3.3
$\text{HPO}_4^=$	χ_{55}	0.54	1.5	3.2
HS^-	χ_{60}	0.32	1.4	3.2
$\text{S}^=$	χ_{61}	3.6	4.1	5.8
PO_4^-	χ_{62}	2.9	3.2	3.9
CdA_2	χ_{63}	3.3	3.6	3.9
CaPO_4^-	χ_{64}	4.6	4.9	5.6
Fe^{2+}	χ_{72}	0.04	0.04	0.06
FeHPO_4^0	χ_{77}	3.3	3.2	4.0
FeSO_4^0	χ_{80}	2.8	2.8	3.0
Cd(HS)^+	χ_{82}	2.7	3.3	6.7
Hg(OH)_2^0	χ_{85}	9.4	9.0	8.6
HgCl_2^0	χ_{91}	4.6	5.3	7.7
Hg(HS)_2^0	χ_{99}	0.00007	<0.00001	<0.00001
Hg^{+2}	χ_{103}	3.4	3.9	6.7
Mn^{+2}	χ_{179}	0.91	0.91	0.94
Zn^{+2}	χ_{180}	5.1	5.5	6.2

Appendix 1. Equilibrium Constants.

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_1 = \frac{\gamma_{HCO_3^-}}{\gamma_{H_2CO_3^0}}$	$\alpha_1 \cdot \frac{[HCO_3^-] 10^{-pH}}{[H_2CO_3^0]} = K_1$	-6.385	4.124×10^{-7}	5, p. 37
$\alpha_2 = \frac{\gamma_{CO_3^-}}{\gamma_{HCO_3^-}}$	$\alpha_2 \cdot \frac{[CO_3^-] 10^{-pH}}{[HCO_3^-]} = K_2$	4.167 x 10 ⁻¹¹		1, p. 134
$\alpha_3 = \frac{\gamma_{Ca^{+2}}\gamma_{SO_4^{2-}}}{\gamma_{CaSO_4^0}}$	$\alpha_3 \cdot \frac{[Ca^{++}] [SO_4^-]}{[CaSO_4^0]} = K_3$	5.01 x 10 ⁻³		2, p. 136
$\alpha_4 = \frac{\gamma_{Ca^{+2}}\gamma_{CO_3^{2-}}}{\gamma_{CaCO_3^0}}$	$\alpha_4 \cdot \frac{[Ca^{++}] [CO_3^-]}{[CaCO_3^0]} = K_4$	7.08 x 10 ⁻⁴		5, p. 37
$\alpha_5 = \frac{\gamma_{Mg^{+2}}\gamma_{CO_3^{2-}}}{\gamma_{MgCO_3^0}}$	$\alpha_5 \cdot \frac{[Mg^{++}] [CO_3^-]}{[MgCO_3^0]} = K_5$	1.32 x 10 ⁻³		5, p. 37
$\alpha_6 = \gamma_{Ca^{+2}}\gamma_{CO_3^{2-}}$	$\alpha_6 \cdot \frac{[Ca^{++}] [CO_3^-]}{Solid \ CaCO_3 \ (calcite)} = K_6$	-8.330	4.674×10^{-9}	see notes

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_7 = \gamma_{Ca^{+2}} \gamma_{Mg^{+2}} \gamma^2_{CO_3^{-2}}$	$\alpha_7 \cdot \frac{[Mg^{++}] [Ca^{++}] [CO_3^-]^2}{Solid\ MgCa(CO_3)_2\ (dolomite)} = K_7$		2.00×10^{-17}	2, p. 75
$\alpha_8 = \frac{\gamma_{Ca^{+2}} \gamma_{HCO_3^-}}{\gamma_{CaHCO_3^+}}$	$\alpha_8 \cdot \frac{[Ca^{++}] [HCO_3^-]}{[CaHCO_3^+]} = K_8$		1.00×10^{-1}	5, p. 37
$\alpha_9 = \frac{\gamma_{Mg^{+2}} \gamma_{HCO_3^-}}{\gamma_{MgHCO_3^+}}$	$\alpha_9 \cdot \frac{[Mg^{++}] [HCO_3^-]}{[MgHCO_3^+]} = K_9$		1.22×10^{-1}	5, p. 37
$\alpha_{10} = \frac{\gamma_{Mg^{+2}} \gamma_{SO_4^=}}{\gamma_{MgSO_4^0}}$	$\alpha_{10} \cdot \frac{[Mg^{++}] [SO_4^=]}{[MgSO_4^0]} = K_{10}$		5.62×10^{-3}	2, p. 136
$\alpha_{11} = \frac{\gamma_{H_2CO_3}}{P_{CO_2}}$	$\alpha_{11} \cdot \frac{[H_2CO_3]}{P_{CO_2}} = K_{11}$	-1.4025	3.958×10^{-2}	5, p. 37
$\alpha_{12} = 0$	$\alpha_{12} = 0$			

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{13} = \frac{\gamma_{Ca^{+2}}\gamma_{OH^-}}{\gamma_{CaOH^+}}$	$\alpha_{13} \cdot \frac{[Ca^{++}][OH^-]}{[CaOH^+]} = K_{13}$		5.01×10^{-2}	1, p. 42
$\alpha_{14} = \frac{\gamma_{Mg^{+2}}\gamma_{OH^-}}{\gamma_{MgOH^+}}$	$\alpha_{14} \cdot \frac{[Mg^{++}][OH^-]}{[MgOH^+]} = K_{14}$		2.63×10^{-3}	1, p. 42
$\alpha_{15} = \frac{\gamma_{HSO_4^-}}{\gamma_{SO_4^{-2}}}$	$\alpha_{15} \cdot \frac{[HSO_4^-] 10^{pH}}{[SO_4^{=}] } = K_{15}$		8.606×10^1	2, p. 134-135
$\alpha_{16} = \frac{1}{\gamma_{HSO_4^-}}$	$\alpha_{16} \cdot \frac{[H_2SO_4^0] 10^{pH}}{[HSO_4^-]} = K_{16}$	-3.0	1.0×10^{-3}	1, p. 233
$\alpha_{17} = \gamma_{OH^-}$	$\alpha_{17} \cdot [OH^-] 10^{-pH} = K_{17}$		6.757×10^{-15}	5, p. 1
$\alpha_{18} = \frac{\gamma_{CuCO_3^0}}{\gamma_{Cu^{+2}}\gamma_{CO_3^{-2}}}$	$\alpha_{18} \cdot \frac{[CuCO_3^0]}{[Cu^{++}][CO_3^{=}]} = K_{18}$		5.37×10^6	2, p. 77

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{19} = \frac{\gamma_{Cu(CO_3)_2^0}}{\gamma_{Cu^{+2}} \gamma_{CO_3^{-2}}^2}$	$\alpha_{19} \cdot \frac{[Cu(CO_3)_2^-]}{[Cu^{++}][CO_3^-]^2} = K_{19}$		1.023×10^{10}	1, p. 140
$\alpha_{20} = \gamma_{Cu^{+2}}$	$\alpha_{20} \cdot \frac{[Cu^{++}][OH^-]^2}{CuO_{(s)} + H_2O \rightarrow Cu^{++} + 2OH^-} = K_{20}$		4.467×10^{-21}	2, p. 26
$\alpha_{21} = \frac{\gamma_{CuOH^+}}{\gamma_{Cu^{+2}}}$	$\alpha_{21} \cdot \frac{[CuOH^+] 10^{-pH}}{[Cu^{++}]} = K_{21}$		2.015×10^{-8}	5, p. 9
$\alpha_{22} = \frac{\gamma_{Cu(OH)_2^0}}{\gamma_{Cu^{+2}}}$	$\alpha_{22} \cdot \frac{[Cu(OH)_2^0] 10^{-2pH}}{[Cu^{++}]} = K_{22}$		2.09×10^{-14}	1, p. 59
$\alpha_{23} = \frac{\gamma_{Cu(OH)_3^-}}{\gamma_{Cu^{+2}}}$	$\alpha_{23} \cdot \frac{[Cu(OH)_3^-] 10^{-3pH}}{[Cu^{++}]} = K_{23}$		1.58×10^{-27}	3, p. 220
$\alpha_{24} = \frac{\gamma_{Cu(OH)_4^-}}{\gamma_{Cu^{+2}}}$	$\alpha_{24} \cdot \frac{[Cu(OH)_4^-] 10^{-4pH}}{[Cu^{++}]} = K_{24}$		2.51×10^{-40}	5, p. 6

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{25} = \frac{\gamma_{Cu_2(OH)_2^{++}}}{\gamma_{Cu^{+2}}^2}$	$\alpha_{25} \cdot \frac{[Cu_2(OH)_2^{++}] 10^{-2pH}}{[Cu^{++}]^2} = K_{25}$		2.69×10^{-11}	2, p. 26
$\alpha_{26} = \frac{\gamma_{CuSO_4^0}}{\gamma_{SO_4^{-2}} \gamma_{Cu^{+2}}}$	$\alpha_{26} \cdot \frac{[CuSO_4^0]}{[SO_4^-][Cu^{++}]} = K_{26}$		2.24×10^2	2, p. 142
$\alpha_{27} = \frac{\gamma_{CuHCO_3^+}}{\gamma_{Cu^{+2}} \gamma_{CO_3^{-2}}}$	$\alpha_{27} \cdot \frac{[CuHCO_3^+] 10^{pH}}{[Cu^{++}][CO_3^-]} = K_{27}$		2.0×10^{12}	16, p. 198
$\alpha_{28} = \frac{\gamma_{CuCl^+}}{\gamma_{Cu^{+2}} \gamma_{Cl^-}}$	$\alpha_{28} \cdot \frac{[CuCl^+]}{[Cu^{++}][Cl^-]} = K_{28}$		2.5	1, p. 286
$\alpha_{29} = \frac{\gamma_{CuCl_2^0}}{\gamma_{Cu^{+2}} \gamma_{Cl^-}^2}$	$\alpha_{29} \cdot \frac{[CuCl_2^0]}{[Cu^{++}][Cl^-]^2} = K_{29}$		1.3	1, p. 286
$\alpha_{30} = \gamma_{Cu^{+2}} \gamma_{OH^-}^2$	$\alpha_{30} \cdot \frac{[Cu^{++}][OH^-]^2}{Cu(OH)_2(s) \rightarrow Cu^{++} + 2OH^-} = K_{30}$		4.786×10^{-20}	5, p. 6

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{31} = \frac{\gamma_{Cu(NH_3)_1^{++}}}{\gamma_{Cu} \cdot \gamma_{NH_3^0}}$	$\alpha_{31} \cdot \frac{[Cu(NH_3)_1^{++}]}{[Cu^{++}][NH_3]} = K_{31}$		1.10×10^4	5, p. 41
$\alpha_{32} = \frac{\gamma_{Cu(NH_3)_2^{++}}}{\gamma_{Cu} \cdot \gamma_{NH_3^0}^2}$	$\alpha_{32} \cdot \frac{[Cu(NH_3)_2^{++}]}{[Cu^{++}][NH_3]^2} = K_{32}$		2.95×10^7	5, p. 41
$\alpha_{33} = \frac{\gamma_{Cu(NH_3)_3^{++}}}{\gamma_{Cu} \cdot \gamma_{NH_3^0}^3}$	$\alpha_{33} \cdot \frac{[Cu(NH_3)_3^{++}]}{[Cu^{++}][NH_3]^3} = K_{33}$		1.778×10^{10}	5, p. 41
$\alpha_{34} = 1$	$\alpha_{34} \cdot \frac{[CuA_2] 10^{-2pH}}{[HA]^2[Cu^{++}]} = K_{34}$		3.12×10^3 $-1.00 \times 10^{-3}\sqrt{I}$	17, p. 519 18, p. 665
$\alpha_{35} = \frac{\gamma_{NH_4^+}}{\gamma_{NH_3^0}}$	$\alpha_{35} \cdot \frac{[NH_3^0] 10^{-pH}}{[NH_4^+]} = K_{35}$		3.987×10^{-10}	5, p. 40
$\alpha_{36} = \frac{\gamma_{CuAc^-}}{\gamma_{Cu} \cdot \gamma_{Ac^-}}$	$\alpha_{36} \cdot \frac{[CuAc^-]}{[Cu^{++}][Ac^-]} = K_{36}$		1.70×10^2	2, p. 251

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{37} = \frac{\gamma_{Cu(Ac)_2^0}}{\gamma_{Cu^{++}}\gamma_{Ac^-}^2}$	$\alpha_{37} \cdot \frac{[Cu(Ac)_2^0]}{[Cu^{++}][Ac^-]^2} = K_{37}$	4.27 x 10 ³		2, p. 251
$\alpha_{38} = \frac{\gamma_{HAc^0}}{\gamma_{Ac^-}}$	$\alpha_{38} \cdot \frac{[HAc] 10^{pH}}{[Ac^-]} = K_{38}$	5.715 x 10 ⁴		6, p. 3
$\alpha_{39} = \gamma_{Cu^{++}}\gamma_{CO_3^-}$	$\alpha_{39} \cdot \frac{[Cu^{++}][CO_3^-]}{CuCO_{3(s)} \rightarrow Cu^{++} + CO_3^-} = K_{39}$	2.34 x 10 ⁻¹⁰		1, p. 140
$\alpha_{40} = \gamma_{Cd^{++}}\gamma_{OH^-}^2$	$\alpha_{40} \cdot \frac{[Cd^{++}][OH^-]^2}{Cd(OH)_2 solid} = K_{40}$	4.467 x 10 ⁻¹⁵		5, p. 9
$\alpha_{41} = \frac{\gamma_{CdOH^+}}{\gamma_{Cd^{++}}}$	$\alpha_{41} \cdot \frac{[CdOH^+] 10^{-pH}}{[Cd^{++}]} = K_{41}$	7.94 x 10 ⁻¹¹		5, p. 9
$\alpha_{42} = \frac{\gamma_{Cd(OH)_2^0}}{\gamma_{Cd^{++}}}$	$\alpha_{42} \cdot \frac{[Cd(OH)_2^0] 10^{-2pH}}{[Cd^{++}]} = K_{42}$	5.01 x 10 ⁻²¹		5, p. 9

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{43} = \frac{\gamma_{Cd(OH)_3^-}}{\gamma_{Cd^{++}}}$	$\alpha_{43} \cdot \frac{[Cd(OH)_3^-] \cdot 10^{-3pH}}{[Cd^{++}]} = K_{43}$	-33.62	2.40×10^{-34}	5, p. 9
$\alpha_{44} = \frac{\gamma_{Cd(OH)_4^-}}{\gamma_{Cd^{++}}}$	$\alpha_{44} \cdot \frac{[Cd(OH)_4^-] \cdot 10^{-4pH}}{[Cd^{++}]} = K_{44}$	-47.599	2.520×10^{-48}	19, p. 301
$\alpha_{45} = \frac{\gamma_{Cd_2OH^{+++}}}{\gamma_{Cd^{++}}^2}$	$\alpha_{45} \cdot \frac{[Cd_2OH^{+++}] \cdot 10^{-pH}}{[Cd^{++}]^2} = K_{45}$	3.98 x 10 ⁻¹⁰		5, p. 9
$\alpha_{46} = \frac{\gamma_{CdSO_4^0}}{\gamma_{Cd^{++}} \gamma_{SO_4^-}}$	$\alpha_{46} \cdot \frac{[CdSO_4^0]}{[Cd^{++}][SO_4^-]} = K_{46}$	2.88 x 10 ²		5, p. 84
$\alpha_{47} = \frac{\gamma_{CdCl^+}}{\gamma_{Cd^{++}} \gamma_{Cl^-}}$	$\alpha_{47} \cdot \frac{[CdCl^+]}{[Cd^{++}][Cl^-]} = K_{47}$	9.55 x 10 ¹		5, p. 108
$\alpha_{48} = \frac{\gamma_{CdCl_2^0}}{\gamma_{Cd^{++}} \gamma_{Cl^-}^2}$	$\alpha_{48} \cdot \frac{[CdCl_2^0]}{[Cd^{++}][Cl^-]^2} = K_{48}$	3.98 x 10 ²		5, p. 108

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{49} = \frac{\gamma_{CdCl_3^-}}{\gamma_{Cd^{++}}\gamma_{Cl^-}^3}$	$\alpha_{49} \cdot \frac{[CdCl_3^-]}{[Cd^{++}][Cl^-]^3} = K_{49}$	2.51×10^2		5, p. 108
$\alpha_{50} = \frac{\gamma_{Cd(NH_3)_2^{++}}}{\gamma_{Cd^{++}}\gamma_{NH_3^0}}$	$\alpha_{50} \cdot \frac{[Cd(NH_3)_2^{++}]}{[Cd^{++}][NH_3^0]} = K_{50}$	3.55×10^2		5, p. 41
$\alpha_{51} = \frac{\gamma_{Cd(NH_3)_2^{++}}}{\gamma_{Cd^{++}}\gamma_{NH_3^0}^2}$	$\alpha_{51} \cdot \frac{[Cd(NH_3)_2^{++}]}{[Cd^{++}][NH_3^0]^2} = K_{51}$	3.63×10^4		5, p. 41
$\alpha_{52} = \frac{\gamma_{Cd(NH_3)_3^{++}}}{\gamma_{Cd^{++}}\gamma_{NH_3^0}^3}$	$\alpha_{52} \cdot \frac{[Cd(NH_3)_3^{++}]}{[Cd^{++}][NH_3^0]^3} = K_{52}$	7.94×10^5		5, p. 41
$\alpha_{53} = \frac{\gamma_{H_3PO_4^0}}{\gamma_{H_2PO_4^-}}$	$\alpha_{53} \cdot \frac{[H_3PO_4] 10^{pH}}{[H_2PO_4^-]} = K_{53}$	1.349×10^2		5, p. 56
$\alpha_{54} = \frac{\gamma_{H_2PO_4^-}}{\gamma_{HPO_4^{--}}}$	$\alpha_{54} \cdot \frac{[H_2PO_4^-] 10^{pH}}{[HPO_4^{--}]} = K_{54}$	1.654×10^7		5, p. 56

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{55} = \frac{\gamma_{HPO_4^=}}{\gamma_{PO_4^{=3-}}}$	$\alpha_{55} \cdot \frac{[HPO_4^=] 10^{pH}}{[PO_4^{=3-}]} = K_{55}$		2.239×10^{12}	5, p. 56
$\alpha_{56} = \frac{\gamma_{CdAc^+}}{\gamma_{Cd^{++}} \gamma_{Ac^-}}$	$\alpha_{56} \cdot \frac{[CdAc^+]}{[Cd^{++}][Ac^-]} = K_{56}$		8.51×10^1	6, p. 6
$\alpha_{57} = \frac{\gamma_{Cd(Ac)_2^0}}{\gamma_{Cd^{++}} \gamma_{Ac^-}^2}$	$\alpha_{57} \cdot \frac{[Cd(Ac)_2^0]}{[Cd^{++}][Ac^-]^2} = K_{57}$		1.41×10^3	6, p. 6
$\alpha_{58} = \frac{\gamma_{Cd(Ac)_3^-}}{\gamma_{Cd^{++}} \gamma_{Ac^-}^3}$	$\alpha_{58} \cdot \frac{[Cd(Ac)_3^-]}{[Cd^{++}][Ac^-]^3} = K_{58}$		1.48×10^2	6, p. 6
$\alpha_{59} = \frac{\gamma_{H_2S^0}}{\gamma_{HS^-}}$	$\alpha_{59} \cdot \frac{[H_2S] 10^{pH}}{[HS^-]} = K_{59}$		1.293×10^7	5, p. 76
$\alpha_{60} = \frac{\gamma_{HS^-}}{\gamma_{S^=}}$	$\alpha_{60} \cdot \frac{[HS^-] 10^{pH}}{[S^=]} = K_{60}$		9.805×10^{13}	5, p. 76

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{61} = \gamma_{S^=}\gamma_{Cd^{++}}$	$\alpha_{61} \cdot \frac{[Cd^{++}][S^=]}{CdS_{(s)} \rightarrow Cd^{++} + S^=} = K_{61}$	1.00×10^{-27}		5, p. 77
$\alpha_{62} = \gamma_{Cd^{++}}\gamma_{CO_3^=}$	$\alpha_{62} \cdot \frac{[Cd^{++}][CO_3^=]}{CdCO_3_{(s)} \rightarrow Cd^{++} + CO_3^=} = K_{62}$	1.820×10^{-14}		1, p. 140
$\alpha_{63} = \gamma_{Cu^{++}}\gamma_{S^=}$	$\alpha_{63} \cdot \frac{[Cu^{++}][S^=]}{CuS_{(s)} \rightarrow Cu^{++} + S^=} = K_{63}$	7.94×10^{-37}		5, p. 76
$\alpha_{64} = \gamma_{Cu^{++}}^2\gamma_{S^=}$	$\alpha_{64} \cdot \frac{[Cu^+]^2[S^=]}{Cu_2S_{(s)} \rightarrow 2Cu^+ + S^=} = K_{64}$	3.16×10^{-49}		5, p. 76
$\alpha_{65} = \gamma_{Cu^{++}}^2\gamma_{OH^-}^2\gamma_{CO_3^=}$	$\alpha_{65} \cdot \frac{[Cu^{++}]^2[OH^-]^2[CO_3^=]}{Cu_2(OH)_2CO_3_{(s)} \rightarrow 2Cu^{++} + 2OH^- + 2CO_3^=} = K_{65}$	1.660×10^{-34}		1, p. 140
$\alpha_{66} = \gamma_{Cu^{++}}^3\gamma_{OH^-}^2\gamma_{CO_3^=}$	$\alpha_{66} \cdot \frac{[Cu^{++}]^3[OH^-]^2[CO_3^=]^2}{Cu_3(OH)_2(CO_3)_{2(s)} \rightarrow 3Cu^{++} + 2OH^- + 2CO_3^=} = K_{66}$	1.096×10^{-46}		1, p. 140

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{67} = \gamma^3_{Cu^{++}} \gamma^2_{PO_4^{=}}$	$\alpha_{67} \cdot \frac{[Cu^{++}]^3 [PO_4^{=}]^2}{Cu_3(PO_4)_{2(s)} \rightarrow 3Cu^{++} + 2PO_4^{=}} = K_{67}$	1.26×10^{-37}		1, p. 186
$\alpha_{68} = \gamma^3_{Cd^{++}} \gamma^2_{PO_4^{=}}$	$\alpha_{68} \cdot \frac{[Cd^{++}]^3 [PO_4^{=}]^2}{Cd_3(PO_4)_{2(s)} \rightarrow 3Cd^{++} + 2PO_4^{=}} = K_{68}$	2.51×10^{-33}		1, p. 186
$\alpha_{69} = \gamma^4_{Cu^{++}} \gamma_{SO_4^{=2}} \gamma^6_{OH^-}$	$\alpha_{69} \cdot \frac{[Cu^{++}]^4 [SO_4^{=}] [OH^-]^6}{Cu_4SO_4(OH)_{6(s)} \rightarrow 4Cu^{++} + SO_4^{=} + 6OH^-} = K_{69}$	3.31×10^{-69}		7, II-4-H-2
$\alpha_{70} = \gamma^2_{Cu^{++}} \gamma_{Cl^-} \gamma^3_{OH^-}$	$\alpha_{70} \cdot \frac{[Cu^{++}]^2 [Cl^-] [OH^-]^3}{Cu_2(OH)_3Cl_{(s)} \rightarrow 2Cu^{++} + 3OH^- + Cl^-} = K_{70}$	2.88×10^{-35}		7, II-4-H-2
$\alpha_{71} = 1$	$\alpha_{71} \cdot \frac{[CdA_2] 10^{-2pH}}{[HA]^2 [Cd^{++}]} = K_{71}$	5.584×10^{-4} -1.36×10^{-3}		17, p. 519 18, p. 665
$\alpha_{72} = \frac{\gamma_{CaPO^-}}{\gamma_{Ca^{++}} \gamma_{PO_4^{=3}}}$	$\alpha_{72} \cdot \frac{[CaPO^-]}{[Ca^{++}] [PO]} = K_{72}$	2.88×10^6		5, p. 56

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{73} = \frac{\gamma_{CaHPO_4^0}}{\gamma_{Ca^{++}HPO}}$	$\alpha_{73} \cdot \frac{[CaHPO_4^0]}{[Ca^{++}][HPO_4^{\equiv}]} = K_{73}$	550		5, p. 56
$\alpha_{74} = \frac{\gamma_{CaH_2PO_4^+}}{\gamma_{Ca^{++}}\gamma_{PO_4^{-3}}}$	$\alpha_{74} \cdot \frac{[CaH_2PO_4^+]}{[Ca^{++}][H_2PO_4^-]} = K_{74}$	31.9		13, p. 477
$\alpha_{75} = \gamma_{Ca^{++}}^5 \gamma_{PO_4^{-3}} \gamma_{OH^-}$	$\alpha_{75} \cdot \frac{[Ca^{++}]^5 [PO_4^{\equiv}]^3 [OH^-]}{Ca_5(PO_4)_3(OH) solid} = K_{75}$	-58.33	4.7×10^{-59}	13, p. 476
$\alpha_{76} = \gamma_{Ca^{++}} \gamma_{HPO_4^=}$	$\alpha_{76} \cdot \frac{[Ca^{++}][HPO_4^=]}{CaHPO_4 solid} = K_{76}$	-6.58	2.62×10^7	5, p. 56
$\alpha_{77} = \gamma_{Ca^{++}}^3 \gamma_{PO_4^{-3}}^2$	$\alpha_{77} \cdot \frac{[Ca^{++}]^3 [PO_4^{-3}]^2}{Ca_3(PO_4)_2 solid} = K_{77}$	-28.92	1.2×10^{-29}	13, p. 476
$\alpha_{78} = \gamma_{Ca^{++}}^4 \gamma_{PO_4^{-3}}^3 \gamma_{H^+}$	$\alpha_{78} \cdot \frac{[Ca^{++}]^4 [PO_4^{\equiv}]^3 [H^+]}{Ca_4(PO_4)_3 H solid} = K_{78}$	-46.90	1.25×10^{-47}	13, p. 476

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{79} = \frac{\gamma_{MgPO_4^-}}{\gamma_{Mg^{++}}\gamma_{PO_4^{-3}}}$	$\alpha_{79} \cdot \frac{[MgPO_4^-]}{[Mg^{++}][PO_4^{\equiv}]} = K_{79}$	60	1×10^6	File 1 estimate
$\alpha_{80} = \frac{\gamma_{MgHPO_4^0}}{\gamma_{Mg^{++}}\gamma_{HPO_4^{\equiv}}}$	$\alpha_{80} \cdot \frac{[MgHPO_4^0]}{[Mg^{++}][HPO_4^{\equiv}]} = K_{80}$	2.91	813	File 1 estimate
$\alpha_{81} = \frac{\gamma_{MgH_2PO_4^+}}{\gamma_{Mg^{++}}\gamma_{H_2PO_4^-}}$	$\alpha_{81} \cdot \frac{[MgH_2PO_4^+]}{[Mg^{++}][H_2PO_4^-]} = K_{81}$	0.8	6.31	File 1 estimate
$\alpha_{82} = \gamma^5_{Mg^{++}}\gamma^3_{PO_4^{-3}}\gamma_{OH^-}$	$\alpha_{82} \cdot \frac{[Mg^{++}]^5[PO_4^{\equiv}]^3[OH^-]}{Mg_5(PO_4)_3 OH solid} = K_{82}$	-52.0	1×10^{-52}	File 1 estimate
$\alpha_{83} = \gamma_{Mg^{++}}\gamma_{HPO_4^{\equiv}}$	$\alpha_{83} \cdot \frac{[Mg^{++}][HPO_4^{\equiv}]}{MgHPO_4(H_2O)_3 solid} = K_{83}$	-5.82	1.5×10^{-6}	5, p. 56
$\alpha_{84} = \gamma^3_{Mg^{++}}\gamma^2_{PO_4^{-3}}$	$\alpha_{84} \cdot \frac{[Mg^{++}]^3[PO_4^{\equiv}]^2}{Mg_3(PO_4)_2(H_2O)_8 solid} = K_{84}$	-25.20	6.31×10^{-26}	5, p. 56

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{85} = \gamma_{Mg}^4 \gamma_{PO_4^{-3}}^3 \gamma_{H^+}$	$\alpha_{85} \cdot \frac{[Mg^{++}]^4 [PO_4^{-3}]^3 [H^+]}{Mg_4(PO_4)_3 H_{solid}} = K_{85}$	-41.8	1.58×10^{-42}	File 1 estimate
$\alpha_{86} = \frac{\gamma_{FeOH^+}}{\gamma_{Fe^{2+}}}$	$\alpha_{86} \cdot \frac{[FeOH^+] 10^{-pH}}{[Fe^{2+}]} = K_{86}$	-9.664	2.168×10^{-10}	File 2 estimate
$\alpha_{87} = \frac{\gamma_{Fe(OH)_2^0}}{\gamma_{Fe^{2+}}}$	$\alpha_{87} \cdot \frac{[Fe(OH)_2^0] 10^{-2pH}}{[Fe^{2+}]} = K_{87}$	-20.948	1.127×10^{-21}	File 2 estimate
$\alpha_{88} = \frac{\gamma_{Fe(OH)_3^-}}{\gamma_{Fe^{2+}}}$	$\alpha_{88} \cdot \frac{[Fe(OH)_3^-] 10^{-3pH}}{[Fe^{2+}]} = K_{88}$	-32.40	3.953×10^{-33}	File 2 estimate
$\alpha_{89} = \frac{\gamma_{Fe(OH)_4^{2-}}}{\gamma_{Fe^{2+}}}$	$\alpha_{89} \cdot \frac{[Fe(OH)_4^{2-}]}{[Fe^{2+}] [OH^-]^4} = K_{89}$	3.981 x 10 ⁹		5, p. 5
$\alpha_{90} = \frac{\gamma_{FeSO_4^0}}{\gamma_{Fe^{2+}} \gamma_{SO_4^{2-}}}$	$\alpha_{90} \cdot \frac{[FeSO_4^0]}{[Fe^{2+}] [SO_4^{2-}]} = K_{90}$	1.585 x 10 ²		5, p. 82

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{91} = \frac{\gamma_{FeHPO_4^0}}{\gamma_{Fe^{2+}}\gamma_{HPO_4^{2-}}}$	$\alpha_{91} \cdot \frac{[FeHPO_4^0]}{[Fe^{2+}][HPO_4^{2-}]} = K_{91}$	3.981 x 10 ³	5, p. 56	
$\alpha_{92} = \frac{\gamma_{FeH_2PO_4^+}}{\gamma_{Fe^{2+}}\gamma_{H_2PO_4^-}}$	$\alpha_{92} \cdot \frac{[FeH_2PO_4^+]}{[Fe^{2+}][H_2PO_4^-]} = K_{92}$	3.981 x 10 ³	5, p. 56	
$\alpha_{93} = \frac{\gamma_{FeAc^-}}{\gamma_{Fe^{2+}}\gamma_{Ac^-}}$	$\alpha_{93} \cdot \frac{[FeAc^-]}{[Fe^{2+}][Ac^-]} = K_{93}$	2.512 x 10 ¹	5, p. 5	
$\alpha_{94} = \gamma_{Fe^{2+}}\gamma_{S^{2-}}$	$\alpha_{94} \cdot \frac{[Fe^{2+}][S^{2-}]}{[FeS]solid} = K_{94}$	2.081 x 10 ⁻¹⁸	14	
$\alpha_{95} = \gamma_{Fe^{2+}}\gamma_{OH^-}^2$	$\alpha_{95} \cdot \frac{[Fe^{2+}][OH^-]^2}{[Fe(OH)_2]solid} = K_{95}$	6.927 x 10 ⁻¹⁶	5, p. 5	
$\alpha_{96} = \gamma_{Fe^{2+}}^3\gamma_{PO_4^{3-}}^2$	$\alpha_{96} \cdot \frac{[Fe^{2+}]^3[PO_4^{3-}]^2}{[Fe_3(PO_4)_2(H_2O)_8]solid} = K_{96}$	1.116 x 10 ⁻³⁶	5, p. 57	

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{97} = \gamma_{Fe^{2+}} \gamma_{CO_3^{2-}}$	$\alpha_{97} \cdot \frac{[Fe^{2+}][CO_3^{2-}]}{[FeCO_3]_{solid}} = K_{97}$	2.484×10^{-11}		5, p. 37
$\alpha_{98} = \frac{\gamma_{Cd(HS^+)}}{\gamma_{Cd^{2+}} \gamma_{HS^-}}$	$\alpha_{98} \cdot \frac{[CdHS^+]}{[Cd^{2+}][HS^-]} = K_{98}$	3.82×10^7		5, p. 77

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{99} = \frac{\gamma_{[Cd(HS)_2^0]}}{\gamma_{[Cd^{2+}]}\gamma_{[HS^-]}}$	$\alpha_{99} \cdot \frac{[Cd(HS)_2^0]}{[Cd^{2+}][HS^-]^2} = K_{99}$		7.59×10^{14}	5, p. 77
$\alpha_{100} = \frac{\gamma_{[Cd(HS)_3^-]}}{\gamma_{[Cd^{2+}]}\gamma_{[HS^-]}^3}$	$\alpha_{100} \cdot \frac{[Cd(HS)_3^-]}{[Cd^{2+}][HS^-]^3} = K_{100}$		4.368×10^{16}	5, p. 77
$\alpha_{101} = \frac{\gamma_{(HgOH^+)}}{\gamma_{Hg^{2+}}\gamma_{OH^-}}$	$\alpha_{101} \cdot \frac{[HgOH^+]}{[Hg^{2+}][OH^-]} = K_{101}$		3.98×10^{10}	5, p. 9
$\alpha_{102} = \frac{\gamma_{Hg(OH)_2^-}}{\gamma_{Hg^{2+}}\gamma_{OH^-}^2}$	$\alpha_{102} \cdot \frac{[Hg(OH)_2^-]}{[Hg^{2+}][OH^-]^2} = K_{102}$		6.31×10^{21}	5, p. 9
$\alpha_{103} = \frac{\gamma_{Hg(OH)_3^-}}{\gamma_{Hg^{2+}}\gamma_{OH^-}^3}$	$\alpha_{103} \cdot \frac{[Hg(OH)_3^-]}{[Hg^{2+}][OH^-]^3} = K_{103}$		7.94×10^{20}	5, p. 9
$\alpha_{104} = \frac{\gamma_{Hg_2OH^{+3}}}{\gamma_{Hg^{2+}}^2\gamma_{OH^-}}$	$\alpha_{104} \cdot \frac{[Hg_2(OH)^{+3}]}{[Hg^{2+}]^2[OH^-]} = K_{104}$		5.01×10^{10}	5, p. 9

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{105} = \frac{\gamma_{Hg_3(OH)_2^{+3}}}{\gamma_{Hg^{+2}}^3 \gamma_{OH^-}^3}$	$\alpha_{105} \cdot \frac{[Hg_3(OH)_3^{+3}]}{[Hg^{+2}]^3 [OH^-]^3} = K_{105}$		3.98×10^{35}	5, p. 9
$\alpha_{106} = \frac{\gamma_{Hg(OH)Cl}}{\gamma_{Hg^{+2}} \gamma_{OH^-} \gamma_{Cl^-}}$	$\alpha_{106} \cdot \frac{[Hg(OH)Cl]}{[Hg^{+2}] [OH^-] [Cl^-]} = K_{106}$		1.41×10^{-9}	File 3 estimate
$\alpha_{107} = \frac{\gamma_{HgCl^+}}{\gamma_{Hg^{+2}} \gamma_{Cl^-}}$	$\alpha_{107} \cdot \frac{[HgCl^+]}{[Hg^{+2}] [Cl^-]} = K_{107}$		5.25×10^3	File 3 estimate
$\alpha_{108} = \frac{\gamma_{HgCl_2^-}}{\gamma_{Hg^{+2}} \gamma_{Cl^-}^2}$	$\alpha_{108} \cdot \frac{[HgCl_2^-]}{[Hg^{+2}] [Cl^-]^2} = K_{108}$		8.71×10^{12}	File 3 estimate
$\alpha_{109} = \frac{\gamma_{HgCl_3^-}}{\gamma_{Hg^{+2}} \gamma_{Cl^-}^3}$	$\alpha_{109} \cdot \frac{[HgCl_3^-]}{[Hg^{+2}] [Cl^-]^3} = K_{109}$		1.0×10^{14}	File 3 estimate
$\alpha_{110} = \frac{\gamma_{Hg(NH_3)^{+2}}}{\gamma_{Hg^{+2}} \gamma_{NH_3^0}}$	$\alpha_{110} \cdot \frac{[Hg(NH_3)^{+2}]}{[Hg^{+2}] [NH_3]} = K_{110}$		4.37×10^8	File 4 estimate

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{111} = \frac{\gamma_{Hg(NH_3)_2^+}}{\gamma_{Hg}^{+2}\gamma_{NH_3^-}^2}$	$\alpha_{111} \cdot \frac{[Hg(NH_3)_2^+]^2}{[Hg]^{+2}[NH_3^-]^2} = K_{111}$		1.10×10^{17}	File 4 estimate
$\alpha_{112} = \frac{\gamma_{Hg(NH_3)_3^+}}{\gamma_{Hg}^{+2}\gamma_{NH_3^-}^3}$	$\alpha_{112} \cdot \frac{[Hg(NH_3)_3^+]^2}{[Hg]^{+2}[NH_3^-]^0} = K_{112}$		7.59×10^{17}	File 4 estimate
$\alpha_{113} = \frac{\gamma_{HgAc^+}}{\gamma_{Hg}^{+2}\gamma_{Ac^-}}$	$\alpha_{113} \cdot \frac{[HgAc^+]^2}{[Hg]^{+2}[Ac^-]} = K_{113}$		1.86×10^5 (30°)	File 5 estimate
$\alpha_{114} = \frac{\gamma_{Hg(Ac)_2^-}}{\gamma_{Hg}^{+2}\gamma_{Ac^-}^2}$	$\alpha_{114} \cdot \frac{[Hg(Ac)_2^-]^0}{[Hg]^{+2}[Ac^-]} = K_{114}$		3.09×10^9 (30°)	File 5 estimate
$\alpha_{115} = \frac{\gamma_{Hg(Ac)_3^-}}{\gamma_{Hg}^{+2}\gamma_{Ac^-}^3}$	$\alpha_{115} \cdot \frac{[Hg(Ac)_3^-]^1}{[Hg]^{+2}[Ac^-]^3} = K_{115}$		3.39×10^{13} (30°)	File 5 estimate
$\alpha_{116} = \frac{\gamma_{Hg(HS)_2^-}}{\gamma_{Hg}^{+2}\gamma_{HS^-}^2}$	$\alpha_{116} \cdot \frac{[Hg(HS)_2^-]^0}{[Hg]^{+2}[HS^-]^2} = K_{116}$		5.45×10^{37} (20°)	5, p. 77

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{117} = \frac{\gamma_{HgSO_4}}{\gamma_{Hg^{+2}}\gamma_{SO_4^{-}}}$	$\alpha_{117} \cdot \frac{[HgSO_4]}{[Hg^{+2}][SO_4^{-2}]} = K_{117}$	1.34	21.88	5, p. 84
$\alpha_{118} = \frac{\gamma_{Hg(SO_4)_2^{-2}}}{\gamma_{Hg^{+2}}\gamma_{SO_4^{-}}^2}$	$\alpha_{118} \cdot \frac{[Hg(SO_4)_2^{-2}]}{[Hg^{+2}][SO_4^{-2}]} = K_{118}$	2.4	2.51×10^2	5, p. 84
$\alpha_{119} = \frac{\gamma_{HgA_2}}{\gamma_{Hg^{+2}}\gamma_{HA}^2}$	$\alpha_{119} \cdot \frac{[HgA_2]}{[Hg^{+2}][HA]^2} = K_{119}$	0.000		File 6 estimate
$\alpha_{120} = \gamma_{Hg^{++}}\gamma_{OH^-}^2$	$\alpha_{120} \cdot \frac{[Hg^{++}][OH^-]^2}{HgO + H_2O \rightarrow Hg^{++} + 2OH^- \text{ red solid}} = K_{120}$	-25.70	1.983×10^{-26}	5, p. 9
$\alpha_{121} = \gamma_{Hg^{++}}\gamma_{S^=}$	$\alpha_{121} \cdot \frac{[Hg^{++}][S^=]}{HgS_{(s)} \text{ black (Metacinnabar)}} = K_{121}$	-53.47	3.379×10^{-54}	5, p. 77
$\alpha_{122} = \gamma_{Hg^{++}}\gamma_{S^=}$	$\alpha_{122} \cdot \frac{[Hg^{++}][S^=]}{HgS_{(s)} \text{ red (Cinnabar)}} = K_{122}$	-54.08	8.746×10^{-55}	5, p. 77

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{123} = \frac{\gamma_{HSeO_3^-}}{\gamma_{SeO_3^=}}$	$\alpha_{123} \cdot \frac{[HSeO_3^-] 10^{pH}}{[SeO_3^=]} = K_{123}$	8.03	1.07×10^8	5, p. 91
$\alpha_{124} = \frac{1}{\gamma_{HSeO_3^-}}$	$\alpha_{124} \cdot \frac{[H_2SeO_3^0] 10^{pH}}{[HSeO_3^-]} = K_{124}$	2.40	2.51×10^2	5, p. 91
$\alpha_{125} = \frac{\gamma_{H_2(SeO_3)_2^{2-}}}{\gamma_{HSeO_3^-}^2}$	$\alpha_{125} \cdot \frac{[H_2(SeO_3)_2^{2-}]}{[HSeO_3^-]^2} = K_{125}$	2.20	1.58×10^2	5, p. 91
$\alpha_{126} = \frac{\gamma_{H_2(SeO_3)_2^{2-}}}{\gamma_{H(SeO_3)_2^{3-}}}$	$\alpha_{126} \cdot \frac{[H_2(SeO_3)_2^{2-}] 10^{pH}}{[H(SeO_3)_2^{3-}]} = K_{126}$	8.12	1.38×10^8	5, p. 91
$\alpha_{127} = \frac{\gamma_{Hg(SeO_3)_2^{2-}}}{\gamma_{Hg^{++}} \gamma_{SeO_3^=}}$	$\alpha_{127} \cdot \frac{[Hg(SeO_3)_2^{2-}]}{[Hg^{++}][SeO_3^{2-}]} = K_{127}$	12.91	8.13×10^{12}	5, p. 91
$\alpha_{128} = \frac{\gamma_{Cd(SeO_3)_2^{2-}}}{\gamma_{Cd^{++}} \gamma_{SeO_3^=}^2}$	$\alpha_{128} \cdot \frac{[Cd(SeO_3)_2^{2-}]}{[Cd^{++}][SeO_3^{2-}]^2} = K_{128}$	5.14	1.37×10^5	5, p. 91

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{129} = \gamma_{Hg^{++}} \gamma_{SeO_3^-}$	$\alpha_{129} \cdot \frac{[Hg^{++}][SeO_3^-]}{HgSeO_3(s)} = K_{129}$	-13.86	1.39×10^{-14}	5, p. 91
$\alpha_{130} = \gamma_{Cu^{++}} \gamma_{SeO_3^-}$	$\alpha_{130} \cdot \frac{[Cu^{++}][SeO_3^-]}{CuSeO_3(s)} = K_{130}$	-7.78 (at 20°C)	1.66×10^{-8}	5, p. 91
$\alpha_{131} = \gamma_{Mg^{++}} \gamma_{SeO_3^2-}$	$\alpha_{131} \cdot \frac{[Mg^{++}][SeO_3^2-]}{MgSeO_3(s)} = K_{131}$	-5.36 (at 20°C)	4.37×10^{-6}	5, p. 91
$\alpha_{132} = \frac{\gamma_{MnOH^+}}{\gamma_{Mn^{++}} \gamma_{OH^-}}$	$\alpha_{132} \cdot \frac{[MnOH^+]}{[Mn^{++}][OH^-]} = K_{132}$	3.4	2.51×10^3	5, p. 5
$\alpha_{133} = \frac{\gamma_{Mn(OH)_4^{2-}}}{\gamma_{Mn^{++}} \gamma_{OH^-}^4}$	$\alpha_{133} \cdot \frac{[Mn(OH)_4^{2-}]}{[Mn^{++}][OH^-]^4} = K_{133}$	7.7	5.01×10^7	5, p. 5
$\alpha_{134} = \frac{\gamma_{Mn_2(OH)^{3+}}}{\gamma_{Mn}^2 \gamma_{OH^-}}$	$\alpha_{134} \cdot \frac{[Mn_2(OH)^{3+}]}{[Mn^{2+}]^2 [OH^-]} = K_{134}$	3.4	2.51×10^3	5, p. 5

Appendix 1. (cont'd).

DEFINITION	DEFINITION K.	$\log_{10}K$	K	*Ref.
$\alpha_{135} = \frac{\gamma_{Mn_2(OH)_3^+}}{\gamma_{Mn^{2+}}^2 \gamma_{OH^-}^3}$	$\alpha_{135} \cdot \frac{[Mn_2(OH)_3^+]}{[Mn^{2+}]^2 [OH^-]^3} = K_{135}$	18.1	1.26×10^{18}	5, p. 5
$\alpha_{136} = \frac{\gamma_{Mn(HCO_3)^+}}{\gamma_{Mn^{2+}} \gamma_{HCO_3^-}}$	$\alpha_{136} \cdot \frac{[Mn(HCO_3)^+]}{[Mn^{2+}] [HCO_3^-]} = K_{136}$	1.8	63.1	5, p. 37
$\alpha_{137} = \frac{\gamma_{MnSO_4^0}}{\gamma_{Mn^{2+}} \gamma_{SO_4^{2-}}}$	$\alpha_{137} \cdot \frac{[MnSO_4^0]}{[Mn^{2+}] [SO_4^{2-}]} = K_{137}$	2.22	1.656×10^2	5, p. 82
$\alpha_{138} = \frac{\gamma_{MnCl^+}}{\gamma_{Mn^{2+}} \gamma_{Cl^-}}$	$\alpha_{138} \cdot \frac{[MnCl^+]}{[Mn^{2+}] [Cl^-]} = K_{138}$.042	1.10	5, p. 105
$\alpha_{139} = \frac{\gamma_{MnAc^+}}{\gamma_{Mn^{2+}} \gamma_{Ac^-}}$	$\alpha_{139} \cdot \frac{[MnAc^+]}{[Mn^{2+}] [Ac^-]} = K_{139}$	1.40	25.1	6, p. 5
$\alpha_{140} = \frac{\gamma_{MnNH_3^{2+}}}{\gamma_{Mn^{2+}} \gamma_{NH_3}}$	$\alpha_{140} \cdot \frac{[MnNH_3^{2+}]}{[Mn^{2+}] [NH_3]} = K_{140}$	1.00 (20°, 2.0)	10.0	5, p. 40

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{141} = \frac{\gamma_{Mn(NH_3)_2^{2+}}}{\gamma_{Mn^{2+}} \gamma^2_{NH_3}}$	$\alpha_{141} \cdot \frac{[Mn(NH_3)_2^{2+}]}{[Mn^{2+}][NH_3]^2} = K_{141}$	1.54 (20°, 2.0)	34.7	5, p. 40
$\alpha_{142} = \frac{\gamma_{Mn(NH_3)_3^{2+}}}{\gamma_{Mn^{2+}} \gamma^3_{NH_3}}$	$\alpha_{142} \cdot \frac{[Mn(NH_3)_3^{2+}]}{[Mn^{2+}][NH_3]^3} = K_{142}$	1.70 (20°, 2.0)	50.1	5, p. 40
$\alpha_{143} = \frac{\gamma_{Zn(OH)^+}}{\gamma_{Zn^{2+}} \gamma_{OH^-}}$	$\alpha_{143} \cdot \frac{[Zn(OH)^+]}{[Zn^{2+}][OH^-]} = K_{143}$	5.0 ± 0.0	1.0×10^5	5, p. 9
$\alpha_{144} = \frac{\gamma_{Zn(OH)_2^0}}{\gamma_{Zn^{2+}} \gamma^2_{OH^-}}$	$\alpha_{144} \cdot \frac{[Zn(OH)_2^0]}{[Zn^{2+}][OH^-]^2} = K_{144}$	11.1	1.26×10^{11}	5, p. 9
$\alpha_{145} = \frac{\gamma_{Zn(OH)_3^-}}{\gamma_{Zn^{2+}} \gamma^3_{OH^-}}$	$\alpha_{145} \cdot \frac{[Zn(OH)_3^-]}{[Zn^{2+}][OH^-]^3} = K_{145}$	13.6	3.98×10^{13}	5, p. 9
$\alpha_{146} = \frac{\gamma_{Zn_2(OH)^{3+}}}{\gamma^2_{Zn^{2+}} \gamma_{OH^-}}$	$\alpha_{146} \cdot \frac{[Zn_2(OH)^{3+}]}{[Zn^{2+}]^2[OH^-]} = K_{146}$	5.0	1.0×10^5	5, p. 9

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{147} = \frac{\gamma_{Zn(HPO_4)^0}}{\gamma_{Zn^{2+}} \gamma_{HPO_4^{2-}}}$	$\alpha_{147} \cdot \frac{[Zn(HPO_4)^0]}{[Zn^{2+}][HPO_4^{2-}]} = K_{147}$	2.4 (I = 0.1)	2.51×10^2	5, p. 57
$\alpha_{148} = \frac{\gamma_{ZnH_2PO_4^+}}{\gamma_{Zn^{2+}} \gamma_{H_2PO_4^-}}$	$\alpha_{148} \cdot \frac{[ZnH_2PO_4^+]}{[Zn^{2+}][H_2PO_4^-]} = K_{148}$	2.83 (37°)	6.76×10^2	5, p. 57
$\alpha_{149} = \frac{\gamma_{ZnSO_4^0}}{\gamma_{Zn^{2+}} \gamma_{SO_4^{2-}}}$	$\alpha_{149} \cdot \frac{[ZnSO_4^0]}{[Zn^{2+}][SO_4^{2-}]} = K_{149}$	2.38	2.40×10^2	5, p. 84
$\alpha_{150} = \frac{\gamma_{Zn(SO_4)_2^{2-}}}{\gamma_{Zn^{2+}} \gamma_{SO_4^{2-}}^2}$	$\alpha_{150} \cdot \frac{[Zn(SO_4)_2^{2-}]}{[Zn^{2+}][SO_4^{2-}]^2} = K_{150}$	2.6	3.98×10^2	5, p. 84
$\alpha_{151} = \frac{\gamma_{Zn(SO_4)_3^{4-}}}{\gamma_{Zn^{2+}} \gamma_{SO_4^{2-}}^3}$	$\alpha_{151} \cdot \frac{[Zn(SO_4)_3^{4-}]}{[Zn^{2+}][SO_4^{2-}]^3} = K_{151}$	1.5	31.6	5, p. 84
$\alpha_{152} = \frac{\gamma_{ZnCl^+}}{\gamma_{Zn^{2+}} \gamma_{Cl^-}}$	$\alpha_{152} \cdot \frac{[ZnCl^+]}{[Zn^{2+}][Cl^-]} = K_{152}$	0.43	2.69	5, p. 108

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{153} = \frac{\gamma_{Zn(Cl)_2^0}}{\gamma_{Zn^{2+}}\gamma_{Cl^-}^2}$	$\alpha_{153} \cdot \frac{[Zn(Cl)_2^0]}{[Zn^{2+}][Cl^-]^2} = K_{153}$	1.25	17.8	5, p. 108
$\alpha_{154} = \frac{\gamma_{Zn(Cl)_3^-}}{\gamma_{Zn^{2+}}\gamma_{Cl^-}^3}$	$\alpha_{154} \cdot \frac{[Zn(Cl)_3^-]}{[Zn^{2+}][Cl^-]^3} = K_{154}$	0.5	3.16	5, p. 108
$\alpha_{155} = \frac{\gamma_{ZnAc^+}}{\gamma_{Zn^{2+}}\gamma_{Ac^-}}$	$\alpha_{155} \cdot \frac{[ZnAc^+]}{[Zn^{2+}][Ac^-]} = K_{155}$	1.57	37.2	6, p. 6
$\alpha_{156} = \frac{\gamma_{Zn(Ac)_2^0}}{\gamma_{Zn^{2+}}\gamma_{Ac^-}^2}$	$\alpha_{156} \cdot \frac{[Zn(Ac)_2^0]}{[Zn^{2+}][Ac^-]^2} = K_{156}$	1.36 (25°, 3.0)	22.9	6, p. 6
$\alpha_{157} = \frac{\gamma_{Zn(Ac)_3^-}}{\gamma_{Zn^{2+}}\gamma_{Ac^-}^3}$	$\alpha_{157} \cdot \frac{[Zn(Ac)_3^-]}{[Zn^{2+}][Ac^-]^3} = K_{157}$	1.92	83.2	6, p. 6
$\alpha_{158} = \frac{\gamma_{Zn(NH_3)^{2+}}}{\gamma_{Zn^{2+}}\gamma_{NH_3}}$	$\alpha_{158} \cdot \frac{[Zn(NH_3)^{2+}]}{[Zn^{2+}][NH_3]} = K_{158}$	2.21	1.62×10^2	5, p. 41

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{159} = \frac{\gamma_{Zn(NH_3)_2^{2+}}}{\gamma_{Zn^{2+}} \gamma^3_{NH_3}}$	$\alpha_{159} \cdot \frac{[Zn(NH_3)_2^{2+}]}{[Zn^{2+}][NH_3]^2} = K_{159}$	4.50	3.16×10^4	5, p. 41
$\alpha_{160} = \frac{\gamma_{Zn(NH_3)_3^{2+}}}{\gamma_{Zn^{2+}} \gamma^3_{NH_3}}$	$\alpha_{160} \cdot \frac{[Zn(NH_3)_3^{2+}]}{[Zn^{2+}][NH_3]^3} = K_{160}$	6.86	7.24×10^6	5, p. 41
$\alpha_{161} = \frac{\gamma_{Zn(HS)(OH)_0}}{\gamma_{Zn^{2+}} \gamma_{HS^{-1}} \gamma_{OH^{-1}}}$	$\alpha_{161} \cdot \frac{[Zn(HS)(OH)^0]}{[Zn^{2+}][SH^-][OH^-]} = K_{161}$	20.88 (I = 1.0)	7.669×10^{20}	5, p. 76
$\alpha_{162} = \frac{\gamma_{Na(OH)^0}}{\gamma_{Na^+} \gamma_{OH^-}}$	$\alpha_{162} \cdot \frac{[Na(OH)^0]}{[Na^+][OH^-]} = K_{162}$	-0.2	0.63	5, p. 1
$\alpha_{163} = \frac{\gamma_{NaHPO_4^-}}{\gamma_{Na^+} \gamma_{HPO_4^{2-}}}$	$\alpha_{163} \cdot \frac{[NaHPO_4^-]}{[Na^+][HPO_4^{2-}]} = K_{163}$	1.40	25.1	5, p. 56
$\alpha_{164} = \frac{\gamma_{NaSO_4^-}}{\gamma_{Na^+} \gamma_{SO_4^{2-}}}$	$\alpha_{164} \cdot \frac{[NaSO_4^-]}{[Na^+][SO_4^{2-}]} = K_{164}$	0.70 ± 0.05	5.01	5, p. 79

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{165} = \frac{\gamma_{NaAc^0}}{\gamma_{Na^+}\gamma_{Ac^-}}$	$\alpha_{165} \cdot \frac{[NaAc^0]}{[Na^+][Ac^-]} = K_{165}$	-0.18	0.66	6, p. 3
$\alpha_{166} = \frac{\gamma_{KOH^0}}{\gamma_{K^+}\gamma_{OH^-}}$	$\alpha_{166} \cdot \frac{[KOH^0]}{[K^+][OH^-]} = K_{166}$	-0.5	0.32	5, p. 1
$\alpha_{167} = \frac{\gamma_{KHPO_4^-}}{\gamma_{K^+}\gamma_{HPO_4^{2-}}}$	$\alpha_{167} \cdot \frac{[KHPO_4^-]}{[K^+][HPO_4^{2-}]} = K_{167}$	1.195	15.7	5, p. 56
$\alpha_{168} = \frac{\gamma_{KSO_4^-}}{\gamma_{K^+}\gamma_{SO_4^{2-}}}$	$\alpha_{168} \cdot \frac{[KSO_4^-]}{[K^+][SO_4^{2-}]} = K_{168}$	0.85 ± 0.1	7.08	5, p. 79
$\alpha_{169} = \frac{\gamma_{KCl^0}}{\gamma_{K^+}\gamma_{Cl^-}}$	$\alpha_{169} \cdot \frac{[KCl^0]}{[K^+][Cl^-]} = K_{169}$	-0.7	0.20	5, p. 104
$\alpha_{170} = \frac{\gamma_{(Hg_2)OH^+}}{\gamma_{Hg_2^{2+}}\gamma_{OH^-}}$	$\alpha_{170} \cdot \frac{[(Hg_2)OH^+]}{[Hg_2^{2+}][OH^-]} = K_{170}$	17.4	2.51×10^{17}	5, p. 8

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	log ₁₀ K	K	*Ref.
$\alpha_{171} = \frac{\gamma_{(Hg_2)SO_4^0}}{\gamma_{Hg_2^{2+}} \gamma_{SO_4^{2-}}}$	$\alpha_{171} \cdot \frac{[(Hg_2)SO_4^0]}{[Hg_2^{2+}][SO_4^{2-}]} = K_{171}$	5.2	1.58×10^5	5, p. 83
$\alpha_{172} = \frac{\gamma_{(Hg_2)(SO_4)_2^{2-}}}{\gamma_{Hg_2^{2+}} \gamma^2_{SO_4^{2-}}}$	$\alpha_{172} \cdot \frac{[(Hg_2)(SO_4)_2^{2-}]}{[Hg_2^{2+}][SO_4^{2-}]^2} = K_{172}$	7.08	1.20×10^7	5, p. 83
$\alpha_{173} = \frac{\gamma_{Fe(OH)^{2+}}}{\gamma_{Fe^{3+}} \gamma_{OH^-}}$	$\alpha_{173} \cdot \frac{[Fe(OH)^{2+}]}{[Fe^{3+}][OH^-]} = K_{173}$	11.85	7.00×10^{11}	5, p. 7
$\alpha_{174} = \frac{\gamma_{Fe(OH)_2^+}}{\gamma_{Fe^{3+}} \gamma^2_{OH^-}}$	$\alpha_{174} \cdot \frac{[Fe(OH)_2^+]}{[Fe^{3+}][OH^-]^2} = K_{174}$	22.3	2.0×10^{22}	5, p. 7
$\alpha_{175} = \frac{\gamma_{(Fe)_2(OH)_2^{4+}}}{\gamma^2_{Fe^{3+}} \gamma^2_{OH^-}}$	$\alpha_{175} \cdot \frac{[(Fe)_2(OH)_2^{4+}]}{[Fe^{3+}]^2[OH^-]^2} = K_{175}$	25.1	1.259×10^{25}	5, p. 7
$\alpha_{176} = \frac{\gamma_{Fe_3(OH)_4^{5+}}}{\gamma^3_{Fe^{3+}} \gamma^4_{OH^-}}$	$\alpha_{176} \cdot \frac{[Fe_3(OH)_4^{5+}]}{[Fe^{3+}]^3[OH^-]^4} = K_{176}$	49.7	5.01×10^{49}	5, p. 7

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{177} = \frac{\gamma_{FeHPO_4^+}}{\gamma_{Fe^{3+}}\gamma_{HPO_4^{2-}}}$	$\alpha_{177} \cdot \frac{[FeHPO_4^+]}{[Fe^{3+}][HPO_4^{2-}]} = K_{177}$	8.30 (I=0.5)	2.00×10^8	5, p. 57
$\alpha_{178} = \frac{\gamma_{FeH_2PO_4^{2+}}}{\gamma_{Fe^{3+}}\gamma_{H_2PO_4^-}}$	$\alpha_{178} \cdot \frac{[FeH_2PO_4^{2+}]}{[Fe^{3+}][H_2PO_4^-]} = K_{178}$	3.47	2.95×10^3	5, p. 57
$\alpha_{179} = \frac{\gamma_{FeSO_4^+}}{\gamma_{Fe^{3+}}\gamma_{SO_4^{2-}}}$	$\alpha_{179} \cdot \frac{[FeSO_4^+]}{[Fe^{3+}][SO_4^{2-}]} = K_{179}$	3.96	9.221×10^3	5, p. 79
$\alpha_{180} = \frac{\gamma_{Fe(SO_4)_2^-}}{\gamma_{Fe^{3+}}\gamma_{SO_4^{2-}}^2}$	$\alpha_{180} \cdot \frac{[Fe(SO_4)_2^-]}{[Fe^{3+}][SO_4^{2-}]^2} = K_{180}$	5.38	2.4×10^5	5, p. 83
$\alpha_{181} = \frac{\gamma_{FeCl^{+2}}}{\gamma_{Fe^{3+}}\gamma_{Cl^-}}$	$\alpha_{181} \cdot \frac{[FeCl^{+2}]}{[Fe^{3+}][Cl^-]} = K_{181}$	1.38	23.884	5, p. 106

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{182} = \frac{\gamma_{Fe(Cl)_2^+}}{\gamma_{Fe^{3+}}\gamma_{Cl^-}^2}$	$\alpha_{182} \cdot \frac{[Fe(Cl)_2^+]}{[Fe^{3+}][Cl^-]^2} = K_{182}$	2.13	1.35×10^2	5, p. 106
$\alpha_{183} = \frac{\gamma_{Fe(Cl)_3^0}}{\gamma_{Fe^{3+}}\gamma_{Cl^-}^3}$	$\alpha_{183} \cdot \frac{[Fe(Cl)_3^0]}{[Fe^{3+}][Cl^-]^3} = K_{183}$	-0.78	0.17	5, p. 106
$\alpha_{184} = \frac{\gamma_{Fe(Ac)^{2+}}}{\gamma_{Fe^{3+}}\gamma_{Ac^-}}$	$\alpha_{184} \cdot \frac{[Fe(Ac)^{2+}]}{[Fe^{3+}][Ac^-]} = K_{184}$	3.41	2.57×10^3	6, p. 5
$\alpha_{185} = \frac{\gamma_{Fe(Ac)_2^+}}{\gamma_{Fe^{3+}}\gamma_{Ac^-}^2}$	$\alpha_{185} \cdot \frac{[Fe(Ac)_2^+]}{[Fe^{3+}][Ac^-]^2} = K_{185}$	6.52	3.31×10^6	6, p. 5
$\alpha_{186} = \frac{\gamma_{Fe(Ac)_3^0}}{\gamma_{Fe^{3+}}\gamma_{Ac^-}^3}$	$\alpha_{186} \cdot \frac{[Fe(Ac)_3^0]}{[Fe^{3+}][Ac^-]^3} = K_{186}$	8.5 (20°, 0.1)	3.16×10^8	6, p. 5
$\alpha_{187} = \frac{\gamma_{FeHSeO_3^{2+}}}{\gamma_{Fe^{3+}}\gamma_{HSeO_3^-}}$	$\alpha_{187} \cdot \frac{[FeHSeO_3^{2+}]}{[Fe^{3+}][HSeO_3^-]} = K_{187}$	2.985	9.66×10^2	5, p. 91

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{188} = \frac{\gamma_{FeHSiO_4^0}}{\gamma_{Fe^{3+}}\gamma_{HSiO_4^{3-}}}$	$\alpha_{188} \cdot \frac{[FeHSiO_4^0]}{[Fe^{3+}][HSiO_4^{3-}]} = K_{188}$	8.9 (25°, 0.1)	7.94×10^8	5, p. 39
$\alpha_{189} = \frac{\gamma_{H_2SiO_4^{2-}}}{\gamma_{HSiO_4^{3-}}}$	$\alpha_{189} \cdot \frac{[H_2SiO_4^{2-}] 10^{pH}}{[HSiO_4^{3-}]} = K_{189}$	9.89	7.76×10^9	20, p. 51
$\alpha_{190} = \frac{\gamma_{HSiO_4^{3-}}}{\gamma_{SiO_4^{4-}}}$	$\alpha_{190} \cdot \frac{[H_2SiO_4^{3-}] 10^{pH}}{[SiO_4^{4-}]} = K_{190}$	13.1	1.26×10^{13}	20, p. 51
$\alpha_{191} = \frac{\gamma_{H_2(SiO_4)_2^{-6}}}{\gamma^2_{SiO_4^{-4}}}$	$\alpha_{191} \cdot \frac{[H_2(SiO_4)_2^{-6}] 10^{2pH}}{[SiO_4^{-4}]^2} = K_{191}$	26.16 (25°, 3.0)	1.45×10^{26}	5, p. 39
$\alpha_{192} = \frac{\gamma_{H_4(SiO_4)_4^{-12}}}{\gamma^4_{SiO_4^{-4}}}$	$\alpha_{192} \cdot \frac{10^{4pH} [H_4(SiO_4)_4^{-12}]}{[SiO_4^{-4}]^4} = K_{192}$	55.9	7.94×10^{55}	5, p. 39
$\alpha_{193} = \frac{\gamma_{H_6(SiO_4)_4^{-10}}}{\gamma^4_{SiO_4^{-4}}}$	$\alpha_{193} \cdot \frac{10^{6pH} [H_6(SiO_4)_4^{-10}]}{[SiO_4^{-4}]^4} = K_{193}$	69.49	3.0698×10^{69}	5, p. 39

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{194} = \frac{\gamma_{MgSiO_4^{2-}}}{\gamma_{Mg^{2+}}\gamma_{SiO_4^{-4}}}$	$\alpha_{194} \cdot \frac{[MgSiO_4^{-2}]}{[Mg^{2+}][SiO_4^{-4}]} = K_{194}$	4.91	8.13×10^4	5, p. 39
$\alpha_{195} = \frac{\gamma_{MgHSiO_4^{-}}}{\gamma_{Mg^{2+}}\gamma_{HSiO_4^{-3}}}$	$\alpha_{195} \cdot \frac{[MgHSiO_4^{-}]}{[Mg^{2+}][HSiO_4^{-3}]} = K_{195}$	0.723	5.28	5, p. 39
$\alpha_{196} = \frac{\gamma_{Mg(HSiO_4)_2^{-4}}}{\gamma_{Mg^{2+}}\gamma_{HSiO_4^{-3}}^2}$	$\alpha_{196} \cdot \frac{[Mg(HSiO_4)_2^{-4}]}{[Mg^{2+}][HSiO_4^{-3}]^2} = K_{196}$	3.71	5.13×10^3	5, p. 39
$\alpha_{197} = \frac{\gamma_{CaSiO_4^{-2}}}{\gamma_{Ca^{+2}}\gamma_{SiO_4^{-4}}}$	$\alpha_{197} \cdot \frac{[CaSiO_4^{-2}]}{[Ca^{+2}][SiO_4^{-4}]} = K_{197}$	3.64	4.37×10^3	5, p. 39
$\alpha_{198} = \frac{\gamma_{CaHSiO_4^{-}}}{\gamma_{Ca^{+2}}\gamma_{HSiO_4^{-3}}}$	$\alpha_{198} \cdot \frac{[CaHSiO_4^{-}]}{[Ca^{+2}][HSiO_4^{-3}]} = K_{198}$	0.44	2.75	5, p. 39
$\alpha_{199} = \frac{\gamma_{Ca(HSiO_4)_2^{-4}}}{\gamma_{Ca^{+2}}\gamma_{HSiO_4^{-3}}^2}$	$\alpha_{199} \cdot \frac{[Ca(HSiO_4)_2^{-4}]}{[Ca^{+2}][HSiO_4^{-3}]^2} = K_{199}$	2.89	7.763×10^2	5, p. 39

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{200} = \gamma_{Mg}^2 \cdot \gamma_{HSiO_4}^3$	$\alpha_{200} \cdot \frac{[Mg^{+2}]^2 [HSiO_4]^4}{[Mg_2(HSiO_4)_3(H_2O)_4]} = K_{200}$	-38.3 (51,0)	1.58×10^{-39}	5, p. 39
$\alpha_{201} = \gamma_{Mn^{2+}} \cdot \gamma_{OH^-}$	$\alpha_{201} \cdot \frac{[Mn^{+2}] [OH^-]^2}{[Mn(OH)_2] solid} = K_{201}$	-12.8 ± 0.1	1.433×10^{-13}	5, p. 5
$\alpha_{202} = \gamma_{Mn^{2+}} \cdot \gamma_{CO_3^{-2}}$	$\alpha_{202} \cdot \frac{[Mn^{+2}] [CO_3^{-2}]}{[MnCo_3] solid} = K_{202}$	-9.26	5.545×10^{-10}	5, p. 37
$\alpha_{203} = \gamma_{Mn^{2+}} \cdot \gamma_{S^{-2}}$	$\alpha_{203} \cdot \frac{[Mn^{+2}] [S^{-2}]}{[MnS] solid (pink)} = K_{203}$	-10.58	2.642×10^{-11}	5, p. 79
$\alpha_{204} = \gamma_{Mn^{2+}} \cdot \gamma_{S^{-2}}$	$\alpha_{204} \cdot \frac{[Mn^{+2}] [S^{-2}]}{[MnS] (solid) green} = K_{204}$	-13.56	2.742×10^{-14}	5, p. 76
$\alpha_{205} = \gamma_{Mn^{2+}} \cdot \gamma_{SeO_3^{-2}}$	$\alpha_{205} \cdot \frac{[Mn^{+2}] [SeO_3^{-2}]}{[MnSeO_3] solid} = K_{205}$	-7.27 (20, 0)	5.37×10^{-8}	5, p. 91

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{206} = \gamma_{Zn^{+2}} \gamma_{OH^-}^2$	$\alpha_{206} \cdot \frac{[Zn^{+2}][OH^-]^2}{[Zn(OH)_2]solid} = K_{206}$	-15.60	2.485×10^{-16}	5, p. 9
$\alpha_{207} = \gamma_{Zn^{+2}} \gamma_{OH^-}^2$	$\alpha_{207} \cdot \frac{[Zn^{+2}][OH^-]^2}{[ZnO]solid} = K_{207}$	-16.72	1.903×10^{-17}	5, p. 9
$\alpha_{208} = \gamma_{Zn^{+2}} \gamma_{CO_3^{-2}}$	$\alpha_{208} \cdot \frac{[Zn^{+2}][CO_3^{-2}]}{[ZnCO_3]solid} = K_{208}$	-10.00	1.0×10^{-10}	5, p. 38
$\alpha_{209} = \gamma_{Zn^{+2}}^3 \gamma_{PO_4^{-3}}$	$\alpha_{209} \cdot \frac{[Zn^{+2}]^3 [PO_4^{-3}]^2}{[Zn_3(PO_4)_2]solid [H_2O]_4} = K_{209}$	-34.93	1.177×10^{-35}	5, p. 57
$\alpha_{210} = \gamma_{Zn^{+2}} \gamma_{S^{-2}}$	$\alpha_{210} \cdot \frac{[Zn^{+2}][S^{-2}]}{[ZnS]solid} = K_{210}$	-22.75	1.795×10^{-23}	5, p. 76
$\alpha_{211} = \gamma_{Ca^{+2}} \gamma_{SiO_4^{-3}}$	$\alpha_{211} \cdot \frac{[Ca^{+2}][SiO_4^{-3}]}{[CaSiO_4]solid} = K_{211}$	-7.2	6.31×10^{-8}	5, p. 39

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{212} = \gamma_{Hg_2^{+2}} \gamma_{Cl^-}^2$	$\alpha_{212} \cdot \frac{[Hg_2^{+2}][Cl^-]^2}{[Hg_2(Cl)_2]_{solid}} = K_{212}$	-17.91 ± 0.03	1.23×10^{-18}	5, p. 107
$\alpha_{213} = \gamma_{Fe^{+3}} \gamma_{OH^-}^3$	$\alpha_{213} \cdot \frac{[Fe^{+3}][OH^-]^3}{[Fe(OH)_3](s)} = K_{213}$	-38.8 ± 0.2	1.58×10^{-39}	5, p. 7
$\alpha_{214} = \gamma_{Fe^{+3}} \gamma_{OH^-}^3$	$\alpha_{214} \cdot \frac{[Fe^{+3}][OH^-]^3}{[Fe(OOH)](s,\alpha)} = K_{214}$	-41.5	3.16×10^{-42}	5, p. 7
$\alpha_{215} = \gamma_{Fe^{+3}} \gamma_{OH^-}^3$	$\alpha_{215} \cdot \frac{[Fe^{+3}][OH^-]^3}{[Fe_2O_3^{0.5}](s,\alpha)} = K_{215}$	-42.7	2.0×10^{-43}	5, p. 7
$\alpha_{216} = \gamma_{Hg_2^{+2}} \gamma_{CO_3^{-2}}$	$\alpha_{216} \cdot \frac{[Hg_2^{+2}][CO_3^{-2}]}{[Hg_2CO_3](s)} = K_{216}$	-16.05	8.91×10^{-17}	5, p. 38
$\alpha_{217} = \gamma_{Fe^{+3}} \gamma_{PO_4^{-3}}$	$\alpha_{217} \cdot \frac{[Fe^{+3}][PO_4^{-3}]}{[FePO_4(H_2O)_2](s)} = K_{217}$	-26.4	3.98×10^{-27}	5, p. 57

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{218} = \gamma_{Hg_2^{+2}} \gamma_{HPO_4^{-2}}$	$\alpha_{218} \cdot \frac{[Hg_2^{+2}][HPO_4^{-2}]}{[Hg_2HPO_4](s)} = K_{218}$	-12.40	3.98×10^{-13}	5, p. 57
$\alpha_{219} = \gamma_{Hg_2^{+2}} \gamma_{SO_4^{-2}}$	$\alpha_{219} \cdot \frac{[Hg_2^{+2}][SO_4^{-2}]}{[Hg_2SO_4](s)} = K_{219}$	-6.13 ± 0.04	7.41×10^{-7}	5, p. 38
$\alpha_{220} = \frac{1}{\gamma_{Zn^{++}} \gamma_{HS^-}^2}$	$\alpha_{220} \cdot \frac{[Zn(HS)_2^0]}{[Zn^{++}][SH^-]^2} = K_{220}$	0		
$\alpha_{221} = \frac{\gamma_{HEDTA^{-3}}}{\gamma_{EDTA^{-4}}}$	$\alpha_{221} \cdot \frac{[HEDTA^{-3}] 10^{pH}}{[EDTA^{-4}]} = K_{221}$	11.01	1.033×10^{11}	15, p. 204
$\alpha_{222} = \frac{\gamma_{H_2EDTA^{-2}}}{\gamma_{HEDTA^{-3}}}$	$\alpha_{222} \cdot \frac{[H_2EDTA^{-2}] 10^{pH}}{[HEDTA^{-3}]} = K_{222}$	6.32	2.090×10^6	15, p. 204
$\alpha_{223} = \frac{\gamma_{H_3EDTA^{-1}}}{\gamma_{H_2EDTA^{-2}}}$	$\alpha_{223} \cdot \frac{[H_3EDTA^{-1}] 10^{pH}}{[H_2EDTA^{-2}]} = K_{223}$	2.98	9.549×10^2	15, p. 204

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{224} = \frac{1}{\gamma_{H_3EDTA^{-3}}}$	$\alpha_{224} \cdot \frac{[H_4EDTA^0] 10^{pH}}{[H_3EDTA^{-3}]} = K_{224}$	2.32	2.09×10^2	15, p. 204
$\alpha_{225} = \frac{\gamma_{NaEDTA^{-3}}}{\gamma_{Na^{+1}}\gamma_{EDTA^{-4}}}$	$\alpha_{225} \cdot \frac{[NaEDTA^{-3}]}{[Na^{+1}][EDTA^{-4}]} = K_{225}$	1.98	95.505	15, p. 204
$\alpha_{226} = \frac{\gamma_{MgEDTA^{-2}}}{\gamma_{Mg^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{226} \cdot \frac{[MgEDTA^{-2}]}{[Mg^{+2}][EDTA^{-4}]} = K_{226}$	9.12	1.318×10^9	15, p. 204
$\alpha_{227} = \frac{\gamma_{MgHEDTA^{-1}}}{\gamma_{MgEDTA^{-2}}}$	$\alpha_{227} \cdot \frac{[MgHEDTA^{-1}] 10^{pH}}{[MgEDTA^{-2}]} = K_{227}$	3.53	3.39×10^3	15, p. 204
$\alpha_{228} = \frac{\gamma_{CaEDTA^{-2}}}{\gamma_{Ca^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{228} \cdot \frac{[CaEDTA^{-2}]}{[Ca^{+2}][EDTA^{-4}]} = K_{228}$	11.00	1.00×10^{11}	15, p. 204
$\alpha_{229} = \frac{\gamma_{CaHEDTA^{-1}}}{\gamma_{CaEDTA^{-2}}}$	$\alpha_{229} \cdot \frac{[CaHEDTA^{-1}] 10^{pH}}{[CaEDTA^{-2}]} = K_{229}$	2.86	7.24×10^2	15, p. 204

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{230} = \frac{\gamma_{FeEDTA^{-1}}}{\gamma_{Fe^{+3}}\gamma_{EDTA^{-4}}}$	$\alpha_{230} \cdot \frac{[FeEDTA^{-1}]}{[Fe^{+3}][EDTA^{-4}]} = K_{230}$	25.42	2.632×10^{25}	15, p. 207
$\alpha_{231} = \frac{1}{\gamma_{FeEDTA^{-1}}}$	$\alpha_{231} \cdot \frac{[FeHEDTA^0] 10^{pH}}{[FeEDTA^{-1}]} = K_{231}$	1.62	4.17×10^1	15, p. 207
$\alpha_{232} = \frac{\gamma_{FeEDTA^{-1}}}{\gamma_{FeOHEDTA^{-2}}}$	$\alpha_{232} \cdot \frac{[FeEDTA^{-1}] 10^{pH}}{[FeOHEDTA^{-2}]} = K_{232}$	7.81	6.460×10^7	15, p. 207
$\alpha_{233} = \frac{\gamma_{FeOHEDTA^{-2}}}{\gamma_{Fe(OH)_2EDTA^{-3}}}$	$\alpha_{233} \cdot \frac{[FeOHEDTA^{-2}] 10^{pH}}{[Fe(OH)_2EDTA^{-3}]} = K_{233}$	9.73	5.37×10^9	15, p. 207
$\alpha_{234} = \frac{\gamma_{FeEDTA^{-1}}}{\gamma^2_{(FeOHEDTA)_2^{-2}}}$	$\alpha_{234} \cdot \frac{[FeEDTA^{-1}] 10^{2pH}}{[(FeOHEDTA)_2^{-4}]} = K_{234}$	12.27 25°	1.873×10^{12}	15, p. 207
$\alpha_{235} = \frac{\gamma_{HgEDTA^{-2}}}{\gamma_{Hg^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{235} \cdot \frac{[HgEDTA^{-2}]}{[Hg^{+2}][EDTA^{-4}]} = K_{235}$	22.02	1.048×10^{22}	15, p. 208

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{236} = \frac{\gamma_{HgHEDTA^{-1}}}{\gamma_{HgEDTA^{-2}}}$	$\alpha_{236} \cdot \frac{[HgHEDTA^{-1}] 10^{pH}}{[HgEDTA^{-2}]} = K_{236}$	3.41	2.57×10^3	15, p. 208
$\alpha_{237} = \frac{\gamma_{HgEDTA^{-2}}}{\gamma_{HgOHEDTA^{-3}}}$	$\alpha_{237} \cdot \frac{[HgEDTA^{-2}] 10^{pH}}{[HgOHEDTA^{-3}]} = K_{237}$	9.43	2.69×10^9	15, p. 208

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{238} = \frac{\gamma_{CdEDTA^{-2}}}{\gamma_{Cd^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{238} \cdot \frac{[CdEDTA^{-2}]}{[Cd^{+2}][EDTA^{-4}]} = K_{238}$	16.78	6.029×10^{16}	15, p. 208
$\alpha_{239} = \frac{\gamma_{CdHEDTA^{-1}}}{\gamma_{CdEDTA^{-2}}}$	$\alpha_{239} \cdot \frac{[CdHEDTA^{-1}] 10^{pH}}{[CdEDTA^{-2}]} = K_{239}$	3.21	1.62×10^3	15, p. 208
$\alpha_{240} = \frac{\gamma_{CuEDTA^{-2}}}{\gamma_{Cu^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{240} \cdot \frac{[CuEDTA^{-2}]}{[Cu^{+2}][EDTA^{-4}]} = K_{240}$	19.12	1.319×10^{19}	15, p. 207
$\alpha_{241} = \frac{\gamma_{CuHEDTA^{-1}}}{\gamma_{CuEDTA^{-2}}}$	$\alpha_{241} \cdot \frac{[CuHEDTA^{-1}] 10^{pH}}{[CuEDTA^{-2}]} = K_{241}$	3.32	2.089×10^3	15, p. 207
$\alpha_{242} = \frac{\gamma_{CuOHEDTA^{-3}}}{\gamma_{CuEDTA^{-2}}\gamma_{OH^{-1}}}$	$\alpha_{242} \cdot \frac{[CuOHEDTA^{-3}]}{[CuEDTA^{-2}][OH^{-1}]} = K_{242}$	2.82	6.608×10^2	15, p. 207

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{243} = \frac{\gamma_{FeEDTA^{-2}}}{\gamma_{Fe^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{243} \cdot \frac{[FeEDTA^{-2}]}{[Fe^{+2}][EDTA^{-4}]} = K_{243}$	14.64	4.366×10^{14}	15, p. 206
$\alpha_{244} = \frac{\gamma_{FeHEDTA^{-1}}}{\gamma_{FeEDTA^{-2}}}$	$\alpha_{244} \cdot \frac{[FeHEDTA^{-1}] 10^{pH}}{[FeEDTA^{-2}]} = K_{244}$	3.05	1.12×10^3	15, p. 206
$\alpha_{245} = \frac{\gamma_{FeEDTA^{-2}}}{\gamma_{FeOHEDTA^{-3}}}$	$\alpha_{245} \cdot \frac{[FeEDTA^{-2}] 10^{pH}}{[FeOHEDTA^{-3}]} = K_{245}$	9.39	2.45×10^9	15, p. 206
$\alpha_{246} = \frac{\gamma_{FeOHEDTA^{-3}}}{\gamma_{Fe(OH)_2EDTA^{-4}}}$	$\alpha_{246} \cdot \frac{[FeOHEDTA^{-3}] 10^{pH}}{[Fe(OH)_2EDTA^{-4}]} = K_{246}$	10.16	1.45×10^{10}	15, p. 206
$\alpha_{247} = \frac{\gamma_{MnEDTA^{-2}}}{\gamma_{Mn^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{247} \cdot \frac{[MnEDTA^{-2}]}{[Mn^{+2}][EDTA^{-4}]} = K_{247}$	14.19	1.549×10^{14}	15, p. 206

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{248} = \frac{\gamma_{MnHEDTA^{-1}}}{\gamma_{MnEDTA^{-2}}}$	$\alpha_{248} \cdot \frac{[MnHEDTA^{-1}] 10^{pH}}{[MnEDTA^{-2}]} = K_{248}$	3.41	2.57×10^3	15, p. 206
$\alpha_{249} = \frac{\gamma_{ZnEDTA^{-2}}}{\gamma_{Zn^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{249} \cdot \frac{[ZnEDTA^{-2}]}{[Zn^{+2}][EDTA^{-4}]} = K_{249}$	16.82	6.609×10^{16}	15, p. 208
$\alpha_{250} = \frac{\gamma_{ZnHEDTA^{-1}}}{\gamma_{ZnEDTA^{-2}}}$	$\alpha_{250} \cdot \frac{[ZnHEDTA^{-1}] 10^{pH}}{[ZnEDTA^{-2}]} = K_{250}$	3.29	1.95×10^3	15, p. 208
$\alpha_{251} = \frac{\gamma_{ZnOHEDTA^{-3}}}{\gamma_{ZnEDTA^{-2}}\gamma_{OH^-}}$	$\alpha_{251} \cdot \frac{[ZnOHEDTA^{-3}]}{[ZnEDTA^{-2}][OH^-]} = K_{251}$	3.32	2.09×10^3	15, p. 208
$\alpha_{252} = \frac{\gamma_{KEDTA^{-3}}}{\gamma_K \cdot \gamma_{EDTA^{-4}}}$	$\alpha_{252} \cdot \frac{[KEDTA^{-3}]}{[K^{+1}][EDTA^{-4}]} = K_{252}$	1.12	13.2	15, p. 204

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{253} = \frac{\gamma_{CoEDTA^{-2}}}{\gamma_{Co^{+2}}\gamma_{EDTA^{-4}}}$	$\alpha_{253} \cdot \frac{[CoEDTA^{-2}]}{[Co^{+2}][EDTA^{-4}]} = K_{253}$	16.63	4.267×10^{16}	5, p. 6
$\alpha_{254} = \frac{\gamma_{CoHEDTA^{-1}}}{\gamma_{CoEDTA^{-2}}}$	$\alpha_{254} \cdot \frac{[CoHEDTA^{-1}] 10^{pH}}{[CoEDTA^{-2}]} = K_{254}$	3.30	2.0×10^3	5, p. 6
$\alpha_{255} = \frac{\gamma_{CoOH^{+1}}}{\gamma_{Co^{+2}}\gamma_{OH^-}}$	$\alpha_{255} \cdot \frac{[CoOH^{+1}]}{[Co^{+2}][OH^-]} = K_{255}$	4.30 25°C	2.0×10^4	5, p. 6
$\alpha_{256} = \frac{1}{\gamma_{Co^{+2}}\gamma_{OH^-}^2}$	$\alpha_{256} \cdot \frac{[Co(OH)_2^0]}{[Co^{+2}][OH^-]^2} = K_{256}$	8.4 25°C	2.51×10^8	5, p. 6
$\alpha_{257} = \frac{\gamma_{Co(OH)_3^{-1}}}{\gamma_{Co^{+2}}\gamma_{OH^-}^3}$	$\alpha_{257} \cdot \frac{[Co(OH)_3^{-1}]}{[Co^{+2}][OH^-]^3} = K_{257}$	9.70 25°C	5.01×10^9	5, p. 6
$\alpha_{258} = \frac{\gamma_{Co(OH)_4^{-2}}}{\gamma_{Co^{+2}}\gamma_{OH^-}^4}$	$\alpha_{258} \cdot \frac{[Co(OH)_4^{-2}]}{[Co^{+2}][OH^-]^4} = K_{258}$	10.20 25°C	1.58×10^{10}	5, p. 6

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{259} = \frac{\gamma_{Co_2OH^{+3}}}{\gamma_{Co^{+2}}^2 \gamma_{OH^-}}$	$\alpha_{259} \cdot \frac{[Co_2OH^{+3}]}{[Co^{+2}]^2 [OH^-]} = K_{259}$	2.70 25°C	5.01×10^2	5, p. 6
$\alpha_{260} = \frac{1}{\gamma_{Co^{+2}} \gamma_{SO_4^{-2}}}$	$\alpha_{260} \cdot \frac{[CoSO_4^0]}{[Co^{+2}] [SO_4^{-2}]} = K_{260}$	2.36 25°C	2.29×10^2	5, p. 82
$\alpha_{261} = \frac{\gamma_{CoNH_3^{+2}}}{\gamma_{Co^{+2}} \gamma_{NH_3}}$	$\alpha_{261} \cdot \frac{[CoNH_3^{+2}]}{[Co^{+2}] [NH_3]} = K_{261}$	2.03	107.17	5, p. 40
$\alpha_{262} = \frac{\gamma_{Co(NH_3)_2^{+2}}}{\gamma_{Co^{+2}} \gamma_{NH_3}^2}$	$\alpha_{262} \cdot \frac{[Co(NH_3)_2^{+2}]}{[Co^{+2}] [NH_3]^2} = K_{262}$	3.5	3.16×10^3	5, p. 40
$\alpha_{263} = \frac{\gamma_{Co(NH_3)_3^{+2}}}{\gamma_{Co^{+2}} \gamma_{NH_3}^3}$	$\alpha_{263} \cdot \frac{[Co(NH_3)_3^{+2}]}{[Co^{+2}] [NH_3]^3} = K_{263}$	4.43	2.69×10^4	5, p. 40

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{264} = \frac{1}{\gamma_{Co^{+2}} \gamma_{HPO_4^{-2}}}$	$\alpha_{264} \cdot \frac{[CoHPO_4^0]}{[Co^{+2}][HPO_4^{-2}]} = K_{264}$	2.18 I=0.1, 25°C	1.51×10^2	5, p. 57
$\alpha_{265} = \frac{\gamma_{CoAc^{+1}}}{\gamma_{Co^{+2}} \gamma_{Ac^-}}$	$\alpha_{265} \cdot \frac{[CoAc^{+1}]}{[Co^{+2}][Ac^-]} = K_{265}$	1.46 25°C	2.88×10^1	16, p. 5
$\alpha_{266} = \frac{\gamma_{NHTA^{-2}}}{\gamma_{NTA^{-3}}}$	$\alpha_{266} \cdot \frac{[HNTA^{-2}] 10^{pH}}{[NTA^{-3}]} = K_{266}$	10.33	2.158×10^{10}	15, p. 139
$\alpha_{267} = \frac{\gamma_{H_2NTA^{-1}}}{\gamma_{HNTA^{-2}}}$	$\alpha_{267} \cdot \frac{[H_2NTA^{-1}] 10^{pH}}{[HNTA^{-2}]} = K_{267}$	2.94	8.71×10^2	15, p. 139
$\alpha_{268} = \frac{\gamma_{H_3NTA^0}}{\gamma_{H_2NTA^{-1}}}$	$\alpha_{268} \cdot \frac{[H_3NTA] 10^{pH}}{[H_2NTA^{-1}]} = K_{268}$	1.80	6.309×10^1	15, p. 139
$\alpha_{269} = \frac{\gamma_{MgNTA^{-1}}}{\gamma_{Mg^{+2}} \gamma_{NTA^{-3}}}$	$\alpha_{269} \cdot \frac{[MgNTA^{-1}]}{[Mg^{+2}][NTA^{-3}]} = K_{269}$	6.55	3.547×10^6	15, p. 139

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{270} = \frac{\gamma_{CaNTA^-}}{\gamma_{Ca^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{270} \cdot \frac{[CaNTA^-]}{[Ca^{+2}][NTA^{-3}]} = K_{270}$	7.61	4.055×10^7	15, p. 139
$\alpha_{271} = \frac{\gamma_{Ca(NTA)_2^{-4}}}{\gamma_{Ca^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{271} \cdot \frac{[Ca(NTA)_2^{-4}]}{[Ca^{+2}][NTA^{-3}]^2} = K_{271}$	10.00	1.00×10^{10}	15, p. 139
$\alpha_{272} = \frac{\gamma_{FeNTA^-}}{\gamma_{Fe^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{272} \cdot \frac{[FeNTA^-]}{[Fe^{+2}][NTA^{-3}]} = K_{272}$	9.47	2.95×10^9	15, p. 141
$\alpha_{273} = \frac{\gamma_{Fe(NTA)_2^{-4}}}{\gamma_{Fe^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{273} \cdot \frac{[Fe(NTA)_2^{-4}]}{[Fe^{+2}][NTA^{-3}]^2} = K_{273}$	14.41	2.57×10^{14}	15, p. 141
$\alpha_{274} = \frac{\gamma_{FeHNTA^-}}{\gamma_{FeNTA^-}}$	$\alpha_{274} \cdot \frac{[FeHNTA^0] 10^{pH}}{[FeNTA^-]} = K_{274}$	3.51	3.24×10^3	15, p. 141
$\alpha_{275} = \frac{\gamma_{FeNTA^-}}{\gamma_{FeOHNTA^{-2}}}$	$\alpha_{275} \cdot \frac{[FeNTA^-] 10^{pH}}{[FeOHNTA^{-2}]} = K_{275}$	11.74	5.5×10^{11}	15, p. 141

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{276} = \frac{\gamma_{CoNTA^-}}{\gamma_{Co^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{276} \cdot \frac{[CoNTA^-]}{[Co^{+2}][NTA^{-3}]} = K_{276}$	11.52	3.31×10^{11}	15, p. 141
$\alpha_{277} = \frac{\gamma_{Co(NTA)_2^{-4}}}{\gamma_{Co^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{277} \cdot \frac{[Co(NTA)_2^{-4}]}{[Co^{+2}][NTA^{-3}]^2} = K_{277}$	15.53	3.389×10^{15}	15, p. 141
$\alpha_{278} = \frac{\gamma_{CoNTA^-}}{\gamma_{CoOHNTA^{-2}}}$	$\alpha_{278} \cdot \frac{[CoNTA^-] 10^{pH}}{[CoOHNTA^{-2}]} = K_{278}$	11.80	6.313×10^{11}	15, p. 141
$\alpha_{279} = \frac{\gamma_{CuNTA^-}}{\gamma_{Cu^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{279} \cdot \frac{[CuNTA^-]}{[Cu^{+2}][NTA^{-3}]} = K_{279}$	14.08	1.2×10^{14}	15, p. 141
$\alpha_{280} = \frac{\gamma_{Cu(NTA)_2^{-4}}}{\gamma_{Cu^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{280} \cdot \frac{[Cu(NTA)_2^{-4}]}{[Cu^{+2}][NTA^{-3}]^2} = K_{280}$	18.50	3.171×10^{18}	15, p. 142
$\alpha_{281} = \frac{\gamma_{CuOHNTA^{-2}}}{\gamma_{CuNTA^-}\gamma_{OH^-}}$	$\alpha_{281} \cdot \frac{[CuOHNTA^{-2}]}{[CuNTA^-][OH^-]} = K_{281}$	5.4 25°C	2.51×10^5	15, p. 142
$\alpha_{282} = 0$	$\alpha_{282} = 0$	0		

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{283} = \frac{1}{\gamma_{Fe^{+3}} \gamma_{NTA^{-3}}}$	$\alpha_{283} \cdot \frac{[FeNTA^0]}{[Fe^{+3}][NTA^{-3}]} = K_{283}$	17.08	1.20×10^{17}	15, p. 142
$\alpha_{284} = \frac{\gamma_{Fe(NTA)_2^{-3}}}{\gamma_{Fe^{+3}} \gamma_{NTA^{-3}}^2}$	$\alpha_{284} \cdot \frac{[Fe(NTA)_2^{-3}]}{[Fe^{+3}][NTA^{-3}]^2} = K_{284}$	25.44	2.75×10^{25}	15, p. 142
$\alpha_{285} = \frac{1}{\gamma_{FeOHNTA^{-1}}}$	$\alpha_{285} \cdot \frac{[FeNTA^0] 10^{pH}}{[FeOHNTA^{-1}]} = K_{285}$	5.24	1.74×10^5	15, p. 142
$\alpha_{286} = \frac{\gamma_{FeOHNTA^{-1}}}{\gamma_{Fe(OH)_2NTA^{-2}}}$	$\alpha_{286} \cdot \frac{[FeOHNTA^{-1}] 10^{pH}}{[Fe(OH)_2NTA^{-2}]} = K_{286}$	8.94	8.71×10^8	15, p. 142
$\alpha_{287} = \frac{\gamma_{ZnNTA^-}}{\gamma_{Zn^{+2}} \gamma_{NTA^{-3}}}$	$\alpha_{287} \cdot \frac{[ZnNTA^-]}{[Zn^{+2}][NTA^{-3}]} = K_{287}$	11.80	6.31×10^{11}	15, p. 142
$\alpha_{288} = \frac{\gamma_{Zn(NTA)_2^{-4}}}{\gamma_{Zn^{+2}} \gamma_{NTA^{-3}}^2}$	$\alpha_{288} \cdot \frac{[Zn(NTA)_2^{-4}]}{[Zn^{+2}][NTA^{-3}]^2} = K_{288}$	15.43	2.692×10^{15}	15, p. 142

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{289} = \frac{\gamma_{ZnOHNTA^{-2}}}{\gamma_{ZnNTA^{-1}}\gamma_{OH^-}}$	$\alpha_{289} \cdot \frac{[ZnOHNTA^{-2}]}{[ZnNTA^-][OH^-]} = K_{289}$	4.56 25°C	3.63×10^4	15, p. 142
$\alpha_{290} = 0$	$\alpha_{290} = 0$		0	
$\alpha_{291} = \frac{\gamma_{CdNTA^-}}{\gamma_{Cd^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{291} \cdot \frac{[CdNTA^-]}{[Cd^{+2}][NTA^{-3}]} = K_{291}$	10.97	9.335×10^{10}	15, p. 142
$\alpha_{292} = \frac{\gamma_{Cd(NTA)_2^{-4}}}{\gamma_{Cd^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{292} \cdot \frac{[Cd(NTA)_2^{-4}]}{[Cd^{+2}][NTA^{-3}]^2} = K_{292}$	15.75	5.626×10^{15}	15, p. 143
$\alpha_{293} = \frac{\gamma_{CdNTA^-}}{\gamma_{CdOHNTA^{-2}}}$	$\alpha_{293} \cdot \frac{[CdNTA^-] 10^{pH}}{[CdOHNTA^{-2}]} = K_{293}$	12.25	1.779×10^{12}	15, p. 143
$\alpha_{294} = \frac{\gamma_{HgNTA^-}}{\gamma_{Hg^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{294} \cdot \frac{[HgNTA^-]}{[Hg^{+2}][NTA^{-3}]} = K_{294}$	15.74 25°C	5.50×10^{15}	15, p. 143

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{295} = \frac{\gamma_{NaNTA^{-2}}}{\gamma_{Na^{+1}}\gamma_{NTA^{-3}}}$	$\alpha_{295} \cdot \frac{[NaNTA^{-2}]}{[Na^{+1}][NTA^{-3}]} = K_{295}$	2.36	2.29×10^2	15, p. 141
$\alpha_{296} = \frac{\gamma_{MnNTA^{-1}}}{\gamma_{Mn^{+2}}\gamma_{NTA^{-3}}}$	$\alpha_{296} \cdot \frac{[MnNTA^{-1}]}{[Mn^{+2}][NTA^{-3}]} = K_{296}$	8.58	3.802×10^8	15, p. 141
$\alpha_{297} = \frac{\gamma_{Mn(NTA)_2^{-4}}}{\gamma_{Mn^{+2}}\gamma_{NTA^{-3}}^2}$	$\alpha_{297} \cdot \frac{[Mn(NTA)_2^{-4}]}{[Mn^{+2}][NTA^{-3}]^2} = K_{297}$	12.13	1.349×10^{12}	15, p. 141
$\alpha_{298} = \gamma_{Co^{+2}}\gamma_{CO_3^{-2}}$	$\alpha_{298} \cdot \frac{[Co^{+2}][CO_3^{-2}]}{[CoCO_3]solid} = K_{298}$	-9.98 25°C	1.05×10^{-10}	5, p. 39
$\alpha_{299} = \gamma_{Co^{+2}}\gamma_{OH^{-1}}^2$	$\alpha_{299} \cdot \frac{[Co^{+2}][OH^{-1}]^2}{[Co(OH)_2]solid} = K_{299}$	-14.9 25°C	1.26×10^{-15}	5, p. 6
$\alpha_{300} = \gamma_{Co^{+2}}^3\gamma_{PO_4^{-3}}^2$	$\alpha_{300} \cdot \frac{[Co^{+2}][PO_4^{-3}]^2}{[Co_3(PO_4)_2]solid} = K_{300}$	-34.7 25°C	2.00×10^{-35}	1, p. 186

Appendix 1 (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{301} = \gamma_{Co^{2+}} \gamma_{S^{-2}}$	$\alpha_{301} \cdot \frac{[Co^{+2}][S^{-2}]}{[CoS]solid} = K_{301}$	-21.3	25°C 5.01×10^{-22}	4, p. 76
$\alpha_{302} = \frac{1}{\gamma_{H_3SiO_4^-}}$	$\alpha_{302} \cdot \frac{[H_4SiO_4^-]}{[H_3SiO_4^-][H^+]} = K_{302}$	9.86	7.2444×10^9	5, p. 39
$\alpha_{303} = \frac{\gamma_{H_3SiO_4^-}}{\gamma_{H_2SiO_4^{-2}}}$	$\alpha_{303} \cdot \frac{[H_3SiO_4^-]}{[H_2SiO_4^{-2}][H^+]} = K_{303}$	13.1	1.25897×10^{13}	5, p. 39

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{304} = 1$	$\alpha_{304} \cdot \frac{[SSCd]}{[SSH_2][Cd^{++}]} = K_{304}$		3.1866×10^{-9}	
$\alpha_{305} = 0$	$\alpha_{305} = 0$			
$\alpha_{306} = 0$	$\alpha_{306} = 0$			
$\alpha_{307} = 0$	$\alpha_{307} = 0$			
$\alpha_{308} = 0$	$\alpha_{308} = 0$			
$\alpha_{309} = 0$	$\alpha_{309} = 0$			
$\alpha_{310} = 0$	$\alpha_{310} = 0$			
$\alpha_{311} = 0$	$\alpha_{311} = 0$			
$\alpha_{312} = 0$	$\alpha_{312} = 0$			

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{313} = 0$	$\alpha_{313} = 0$			
$\alpha_{314} = 0$	$\alpha_{314} = 0$			
$\alpha_{315} = 0$	$\alpha_{315} = 0$			
$\alpha_{316} = 0$	$\alpha_{316} = 0$			
$\alpha_{317} = \frac{\gamma_{AlOH^{+2}}}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{317} \cdot \frac{[AlOH^{+2}]}{[Al^{+3}][OH^-]} = K_{317}$	9.01	1.02×10^9	5, p. 11
$\alpha_{318} = \frac{\gamma_{Al(OH)_2^{+1}}}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{318} \cdot \frac{[Al(OH)_2^{+1}]}{[Al^{+3}][OH^-]^2} = K_{318}$	18.7	5.01×10^{18}	5, p. 11
$\alpha_{319} = \frac{1}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{319} \cdot \frac{[Al(OH)_3]}{[Al^{+3}][OH^-]^3} = K_{319}$	27.0	1.00×10^{27}	5, p. 11

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{320} = \frac{\gamma_{Al(OH)_4^{-1}}}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{320} \cdot \frac{[Al(OH)_4^{-1}]}{[Al^{+3}][OH^-]^4} = K_{320}$	33.0	1.00×10^{33}	5, p. 11
$\alpha_{321} = \frac{\gamma_{Al_2(OH)_2^{+4}}}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{321} \cdot \frac{[Al_2(OH)_2^{+4}]}{[Al^{+3}]^2[OH^-]^2} = K_{321}$	20.3	2.00×10^{20}	5, p. 11
$\alpha_{322} = \frac{\gamma_{Al_3OH_4^{+5}}}{\gamma_{Al^{+3}}\gamma_{OH^-}}$	$\alpha_{322} \cdot \frac{[Al_3(OH)_4^{+5}]}{[Al^{+3}]^3[OH^-]^4} = K_{322}$	42.1	1.26×10^{42}	5, p. 11
$\alpha_{323} = \frac{\gamma_{AlEDTA^{-1}}}{\gamma_{Al^{+3}}\gamma_{EDTA^{-4}}}$	$\alpha_{323} \cdot \frac{[AlEDTA^{-1}]}{[Al^{+3}][EDTA^{-4}]} = K_{323}$	16.3	2.00×10^{16}	15, p. 208
$\alpha_{324} = \frac{\gamma_{AlHEDTA}}{\gamma_{Al^{+3}}\gamma_{EDTA^{-4}}}$	$\alpha_{324} \cdot \frac{[AlHEDTA] \cdot 10^{pH}}{[Al^{+3}][EDTA^{-4}]} = K_{324}$	18.8	6.31×10^{18}	15, p. 208
$\alpha_{325} = \frac{\gamma_{AlOHEDTA^{-2}}}{\gamma_{Al^{+3}}\gamma_{EDTA^{-4}}}$	$\alpha_{325} \cdot \frac{[AlOHEDTA^{-2}]}{[Al^{+3}][EDTA^{-1}]} = K_{325}$	10.41	2.57×10^{10}	15, p. 208

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{326} = \frac{\gamma_{AlNTA^0}}{\gamma_{Al^{+3}}\gamma_{NTA^{-3}}}$	$\alpha_{326} \cdot \frac{[AlNTA^0]}{[Al^{+3}][NTA^{-3}]} = K_{326}$	11.4	2.51×10^{11}	15, p. 208
$\alpha_{327} = \frac{\gamma_{AlHNTA^+}}{\gamma_{Al^{+3}}\gamma_{NTA^{-3}}}$	$\alpha_{327} \cdot \frac{[AlHNTA^+] 10^{pH}}{[Al^{+3}][NTA^{-3}]} = K_{327}$	13.3	2.00×10^{13}	15, p. 143
$\alpha_{328} = \frac{\gamma_{AlOHNTA^+}}{\gamma_{Al^{+3}}\gamma_{NTA^{-3}}}$	$\alpha_{328} \cdot \frac{[AlOHNTA^+] 10^{-pH}}{[Al^{+3}][NTA^{-3}]} = K_{328}$	5.85	7.08×10^5	15, p. 143
$\alpha_{329} = \frac{\gamma_{Al(OH)_2NTA^{-2}}}{\gamma_{Al^{+3}}\gamma_{NTA^{-3}}}$	$\alpha_{329} \cdot \frac{[Al(OH)_2NTA^{-2}]}{[Al^{+3}]^2[NTA^{-3}]} = K_{329}$	-2.96	1.10×10^{-3}	15, p. 143
$\alpha_{330} = \frac{\gamma_{Al(Ac)^{+2}}}{\gamma_{Al^{+3}}\gamma_{Ac^-}}$	$\alpha_{330} \cdot \frac{[Al(Ac)^{+2}]}{[Al^{+3}][Ac^-]} = K_{330}$	1.51	32.36	6, p. 7
$\alpha_{331} = \frac{\gamma_{Al(CO_3)^+}}{\gamma_{Al^{+3}}\gamma_{CO_3^{-2}}}$	$\alpha_{331} \cdot \frac{[Al(CO_3)^+]}{[Al^{+3}][CO_3^{-2}]} = K_{331}$	8.43	2.69×10^8	20, p. 877

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{332} = \frac{\gamma_{AlSO_4^{+1}}}{\gamma_{Al^{+3}}\gamma_{SO_4^{-2}}}$	$\alpha_{332} \cdot \frac{[AlSO_4^{+1}]}{[Al^{+3}][SO_4^{-2}]} = K_{332}$	3.2	1.58×10^3	21, p. 253
$\alpha_{333} = \frac{\gamma_{Al(SO_4)_2^{-1}}}{\gamma_{Al^{+3}}\gamma_{SO_4^{-2}}^2}$	$\alpha_{333} \cdot \frac{[Al(SO_4)_2^{-1}]}{[Al^{+3}][SO_4^{-2}]^2} = K_{333}$	5.1	1.26×10^5	21, p. 253
$\alpha_{334} = \frac{\gamma_{AlH_2PO_4^{+2}}}{\gamma_{Al^{+3}}\gamma_{H_2PO_4^{+1}}}$	$\alpha_{334} \cdot \frac{[AlH_2PO_4^{+2}]}{[Al^{+3}][H_2PO_4^{+1}]} = K_{334}$	10^3	1.00×10^3	1, p. 186
$\alpha_{335} = \frac{\gamma_{Al(H_2PO_4^{+1})_2}}{\gamma_{Al^{+3}}\gamma_{H_2PO_4^{+1}}^2}$	$\alpha_{335} \cdot \frac{[Al(H_2PO_4^{+1})_2]}{[Al^{+3}][H_2PO_4^{+1}]^2} = K_{335}$	5.3	2.00×10^5	1, p. 186
$\alpha_{336} = \frac{\gamma_{Al(H_2PO_4^{+1})_3}}{\gamma_{Al^{+3}}\gamma_{H_2PO_4^{+1}}^3}$	$\alpha_{336} \cdot \frac{[Al(H_2PO_4^{+1})_3]}{[Al^{+3}][N_2PO_4^{-1}]^3} = K_{336}$	7.6	3.98×10^7	1, p. 186
$\alpha_{337} = 1$	$\alpha_{337} \cdot \frac{[AlA_2] \cdot 10^{-2 pH}}{[HA]^2[Al^{+3}]} = K_{337}$	1.37×10^{-2} $-\sqrt{I} * 3.37 \times 10^{-2}$		

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{338} = \gamma_{Al^{+3}} \gamma_{OH^-}^3$	$\alpha_{338} \cdot \frac{[Al^{+3}][OH^-]^3}{[Al(OH)_3] \text{ Gibb site}} = K_{338}$	-33.5	3.16×10^{-34}	5, p. 11
$\alpha_{339} = \gamma_{Al^{+3}} \gamma_{OH^-}^3$	$\alpha_{339} \cdot \frac{Al^{+3}[OH^-]}{[Al(OH)_3] \text{ amorphous}} = K_{339}$	-31.19	6.46×10^{-32}	20
$\alpha_{340} = \gamma_{Al^{+3}} \gamma_{PO_4^{3-}}$	$\alpha_{340} \cdot \frac{[Al^{+3}][PO_4^{3-}]}{[AlPO_4] \text{ solid}} = K_{340}$	-18.24	5.75×10^{-19}	1, p. 186
$\alpha_{341} = \gamma_{Al^{+3}} \gamma_{H_2PO_4^-} \gamma_{OH^-}^2$	$\alpha_{341} \cdot \frac{[Al^{+3}][H_2PO_4^-][OH^-]^2}{[AlH_2PO_4(OH)_2] \text{ solid}} = K_{341}$	-29.55	2.82×10^{-30}	1, p. 186
$\alpha_{342} = \frac{1}{\gamma_{F^-}}$	$\alpha_{342} \cdot \frac{[HF] \cdot 10^{pH}}{[F^-]} = K_{342}$	3.17	1.479×10^3	5, p. 101
$\alpha_{343} = \frac{\gamma_{AlF^{+2}}}{\gamma_{Al^{+3}} \gamma_{F^-}}$	$\alpha_{343} \cdot \frac{[AlF^{+2}]}{[Al^{+3}][F^-]} = K_{343}$	7.0	1.00×10^7	5, p. 101

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{344} = \frac{\gamma_{Al(F)_2^{+1}}}{\gamma_{Al^{+3}}\gamma_{F^{-}}^2}$	$\alpha_{344} \cdot \frac{[Al(F)_2^{+1}]}{[Al^{+3}][F^{-}]^2} = K_{344}$	12.6	3.98×10^{12}	5, p. 101
$\alpha_{345} = \frac{1}{\gamma_{Al^{+3}}\gamma_{F^{-}}^3}$	$\alpha_{345} \cdot \frac{[Al(F)_3^0]}{[Al^{+3}][F^{-}]^3} = K_{345}$	16.7	5.01×10^{16}	5, p. 101
$\alpha_{346} = \frac{\gamma_{Al(F)_4^{-1}}}{\gamma_{Al^{+3}}\gamma_{F^{-}}^4}$	$\alpha_{346} \cdot \frac{[Al(F)_4^{-1}]}{[Al^{+3}][F^{-}]^4} = K_{346}$	19.1	1.259×10^{19}	5, p. 101
$\alpha_{347} = \frac{\gamma_{MgF^{+}}}{\gamma_{Mg^{+2}}\gamma_{F^{-}}}$	$\alpha_{347} \cdot \frac{[MgF^{+1}]}{[Mg^{+2}][F^{-}]} = K_{347}$	1.8	6.31×10^1	
$\alpha_{348} = \frac{\gamma_{CaF^{+}}}{\gamma_{Ca^{+2}}\gamma_{F^{-}}}$	$\alpha_{348} \cdot \frac{[CaF^{+1}]}{[Ca^{+2}][F^{-}]} = K_{348}$	1.1	1.259×10^1	
$\alpha_{349} = \frac{\gamma_{CuF^{+}}}{\gamma_{Cu^{+2}}\gamma_{F^{-}}}$	$\alpha_{349} \cdot \frac{[CuF^{+1}]}{[Cu^{+2}][F^{-}]} = K_{349}$	1.2	1.585×10^1	

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{350} = \frac{\gamma_{HgF^+}}{\gamma_{Hg^{+2}}\gamma_{F^-}}$	$\alpha_{350} \cdot \frac{[HgF^{+1}]}{[Hg^{+2}][F^-]} = K_{350}$	1.6	3.981×10^1	
$\alpha_{351} = \frac{\gamma_{ZnF^+}}{\gamma_{Zn^{+2}}\gamma_{F^-}}$	$\alpha_{351} \cdot \frac{[ZnF^{+1}]}{[Zn^{+2}][F^-]} = K_{351}$	1.15	1.4125×10^1	
$\alpha_{352} = \frac{\gamma_{FeF^{+2}}}{\gamma_{Fe^{+3}}\gamma_{F^-}}$	$\alpha_{352} \cdot \frac{[FeF^{+2}]}{[Fe^{+3}][F^-]} = K_{352}$	6.0	1.000×10^6	
$\alpha_{353} = \frac{\gamma_{FeF_2^+}}{\gamma_{Fe^{+3}}\gamma_{F^-}^2}$	$\alpha_{353} \cdot \frac{[FeF_2^{+1}]}{[Fe^{+3}][F^-]^2} = K_{353}$	10.5	est. 3.16×10^{10}	
$\alpha_{354} = \frac{1}{\gamma_{Fe^{+3}}\gamma_{F^-}^3}$	$\alpha_{354} \cdot \frac{[FeF_3^0]}{[Fe^{+3}][F^-]^3} = K_{354}$	13	est. 1.00×10^{13}	
$\alpha_{355} = \gamma_{Mg^{+2}}\gamma_{F^-}^2$	$\alpha_{355} \cdot \frac{[Mg^{+2}][F^-]^2}{MgF_2 \text{ solid}} = K_{355}$	-8.18	6.607×10^{-9}	

Appendix 1. (cont'd).

DEFINITION	DEFINITION K	$\log_{10}K$	K	*Ref.
$\alpha_{356} = \gamma_{Ca^{+2}} \gamma_F^2$	$\alpha_{356} \cdot \frac{[Ca^{+2}][F^-]^2}{CaF_2 \text{ solid}} = K_{356}$	-10.41	3.8905×10^{-11}	

Appendix 2. Chemical Species and Conversion Factors: M → mg/L of Element.

Species	(χ_i)	Z _i	α_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
CO ₃ ⁼	χ_1	2	4.5	12.01115 x 10 ³	-
HCO ₃ ⁻	χ_2	1	4	12.01115 x 10 ³	-
Ca ⁺⁺	χ_3	2	6	-	40.08 x 10 ³
H ₂ CO ₃	χ_4	0	-	12.01115 x 10 ³	-
Mg ⁺⁺	χ_5	2	8	-	24.312 x 10 ³
SO ₄ ⁼	χ_6	2	4.5	32.064 x 10 ³	-
CaCO ₃ ⁰	χ_7	0	-	12.01115 x 10 ³	40.08 x 10 ³
CaSO ₄ ⁰	χ_8	0	-	32.064 x 10 ³	40.08 x 10 ³
MgCO ₃ ⁰	χ_9	0	-	12.01115 x 10 ³	24.312 x 10 ³
MgSO ₄ ⁰	χ_{10}	0	-	32.064 x 10 ³	24.312 x 10 ³
CaHCO ₃ ⁺	χ_{11}	1	4	12.01115 x 10 ³	40.08 x 10 ³
MgHCO ₃ ⁺	χ_{12}	1	4	12.01115 x 10 ³	24.312 x 10 ³
CaOH ⁺	χ_{13}	1	4	-	40.08 x 10 ³
MgOH ⁺	χ_{14}	1	4	-	24.312 x 10 ³
HSO ₄ ⁻	χ_{15}	1	4	32.064 x 10 ³	-
Cl ⁻	χ_{16}	1	3	35.453 x 10 ³	-
OH ⁻	χ_{17}	1	3.5	-	-
Cu ⁺⁺	χ_{18}	2	6	-	63.54 x 10 ³
CuCO ₃	χ_{19}	0	-	12.01115 x 10 ³	63.54 x 10 ³
Cu(CO ₃) ₂ ⁼	χ_{20}	2	4.5	24.022 x 10 ³	63.54 x 10 ³
Cu(OH) ⁺	χ_{21}	1	4	-	63.54 x 10 ³
Cu(OH) ₂ ⁰	χ_{22}	0	-	-	63.54 x 10 ³
Cu(OH) ₃ ⁻	χ_{23}	1	4	-	63.54 x 10 ³
Cu(OH) ₄ ⁼	χ_{24}	2	4.5	-	63.54 x 10 ³
Cu ₂ (OH) ₂ ⁺⁺	χ_{25}	2	6	-	127.08 x 10 ³
CuSO ₄ ⁰	χ_{26}	0	-	32.064 x 10 ³	63.54 x 10 ³
CuHCO ₃ ⁺	χ_{27}	1	4	12.01115 x 10 ³	63.54 x 10 ³
CuCl ⁺	χ_{28}	1	4	35.453 x 10 ³	63.54 x 10 ³
CuCl ₂ ⁰	χ_{29}	0	-	70.906 x 10 ³	63.54 x 10 ³
CuA ₂	χ_{30}	0	-	355.00 x 10 ³	63.54 x 10 ³
Cu(NH ₃) ⁺⁺	χ_{31}	2	4.5	14.0067 x 10 ³	63.54 x 10 ³
Cu(NH ₃) ₂ ⁺⁺	χ_{32}	2	4.5	28.0134 x 10 ³	63.54 x 10 ³
Cu(NH ₃) ₃ ⁺⁺	χ_{33}	2	4.5	42.0201 x 10 ³	63.54 x 10 ³
NH ₄ ⁺	χ_{34}	1	2.5	14.0067 x 10 ³	-
NH ₃	χ_{35}	0	-	14.0067 x 10 ³	-

Species	(χ_i)	Z_i	\bar{a}_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
CuAc^+	χ_{36}	1	4	24.022×10^3	63.54×10^3
$\text{Cu}(\text{Ac})_2^0$	χ_{37}	0	-	48.045×10^3	63.54×10^3
Ac^-	χ_{38}	1	4.5	24.022×10^3	-
HAc	χ_{39}	0	-	24.022×10^3	-
Cd^{++}	χ_{40}	2	5	-	112.40×10^3
CdOH^+	χ_{41}	1	5	-	112.40×10^3
Cd(OH)_2^0	χ_{42}	0	-	-	112.40×10^3
Cd(OH)_3^-	χ_{43}	1	4.5	-	112.40×10^3
$\text{Cd(OH)}_4^{=}$	χ_{44}	2	5	-	112.40×10^3
$\text{Cd}_2\text{OH}^{+++}$	χ_{45}	3	5	-	224.8×10^3
CdSO_4^0	χ_{46}	0	-	32.064×10^3	112.40×10^3
CdCl^+	χ_{47}	1	4	35.453×10^3	112.40×10^3
CdCl_2^0	χ_{48}	0	-	70.906×10^3	112.40×10^3
CdCl_3^-	χ_{49}	1	5	106.359×10^3	112.40×10^3
$\text{Cd}(\text{NH}_3)^{++}$	χ_{50}	2	5	14.0067×10^3	112.40×10^3
$\text{Cd}(\text{NH}_3)_2^{++}$	χ_{51}	2	5	28.0134×10^3	112.40×10^3
$\text{Cd}(\text{NH}_3)_3^{++}$	χ_{52}	2	5	42.0201×10^3	112.40×10^3
H_3PO_4	χ_{53}	0	-	30.9738×10^3	-
H_2PO_4^-	χ_{54}	1	4.5	30.9738×10^3	-
$\text{HPO}_4^{=}$	χ_{55}	2	4	30.9738×10^3	-
CdAc^+	χ_{56}	1	5	24.022×10^3	112.40×10^3
$\text{Cd}(\text{Ac})_2^0$	χ_{57}	0	-	48.045×10^3	112.40×10^3
$\text{Cd}(\text{Ac})_3^-$	χ_{58}	1	5	72.067×10^3	112.40×10^3
H_2S	χ_{59}	0	-	32.064×10^3	-
HS^-	χ_{60}	1	3.5	32.064×10^3	-
$\text{S}^{=}$	χ_{61}	2	5	32.064×10^3	-
$\text{PO}_4^{=}$	χ_{62}	3	4	30.9738×10^3	-
CdA_2	χ_{63}	0	-	355.00×10^3	112.40×10^3
CaPO_4^-	χ_{64}	1	4	30.9738×10^3	40.08×10^3
CaHPO_4^0	χ_{65}	0	-	30.9738×10^3	40.08×10^3
$\text{CaH}_2\text{PO}_4^+$	χ_{66}	1	4.5	30.9738×10^3	40.08×10^3
MgPO_4^-	χ_{67}	1	4	30.9738×10^3	24.312×10^3
MgHPO_4^0	χ_{68}	0	-	30.9738×10^3	24.312×10^3
$\text{MgH}_2\text{PO}_4^+$	χ_{69}	1	4.5	30.9738×10^3	24.312×10^3
H_2SO_4	χ_{70}	0	-	32.064×10^3	-
HA	χ_{71}	1	-	177.50×10^3	-

Species	(χ_i)	Z_i	\bar{a}_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
Fe^{2+}	χ_{72}	2	6	-	55.847×10^3
FeOH^+	χ_{73}	1	4.5	-	55.847×10^3
Fe(OH)_2^0	χ_{74}	0	-	-	55.847×10^3
Fe(OH)_3^-	χ_{75}	1	4.5	-	55.847×10^3
Fe(OH)_4^{2-}	χ_{76}	2	4.5	-	55.847×10^3
FeHPO_4^0	χ_{77}	0	-	30.9738×10^3	55.847×10^3
$\text{FeH}_2\text{PO}_4^+$	χ_{78}	1	4.5	30.9738×10^3	55.847×10^3
FeAc^+	χ_{79}	1	4.5	24.002×10^3	55.847×10^3
FeSO_4^0	χ_{80}	0	-	32.064×10^3	55.847×10^3
CdHS^+	χ_{81}	1	5	32.064×10^3	112.40×10^3
Cd(HS)_2^0	χ_{82}	0	-	64.13×10^3	112.40×10^3
Cd(HS)_3^-	χ_{83}	1	5	96.19×10^3	112.40×10^3
HgOH^+	χ_{84}	1	4.5	-	200.59×10^3
Hg(OH)_2^0	χ_{85}	0	-	-	200.59×10^3
Hg(OH)_3^-	χ_{86}	1	4.5	-	200.59×10^3
$\text{Hg}_2\text{OH}^{+3}$	χ_{87}	3	4	-	401.18×10^3
$\text{Hg}_3\text{OH}_3^{+3}$	χ_{88}	3	4	-	601.77×10^3
Hg(OH)Cl^0	χ_{89}	0	-	35.453×10^3	200.59×10^3
HgCl^+	χ_{90}	1	4.5	35.453×10^3	200.59×10^3
HgCl_2^0	χ_{91}	0	-	70.91×10^3	200.59×10^3
HgCl_3^-	χ_{92}	1	4.5	106.36×10^3	200.59×10^3
$\text{Hg(NH}_3)_2^{+2}$	χ_{93}	2	5	14.0067×10^3	200.59×10^3
$\text{Hg(NH}_3)_2^{+2}$	χ_{94}	2	5	28.01×10^3	200.59×10^3
$\text{Hg(NH}_3)_3^{+2}$	χ_{95}	2	5	42.02×10^3	200.59×10^3
HgAc^+	χ_{96}	1	4.5	24.022×10^3	200.59×10^3
Hg(Ac)_2^0	χ_{97}	0	-	48.045×10^3	200.59×10^3
Hg(Ac)_3^-	χ_{98}	1	4.5	72.067×10^3	200.59×10^3
Hg(HS)_2^0	χ_{99}	0	-	64.13×10^3	200.59×10^3
HgSO_4^0	χ_{100}	0	-	32.064×10^3	200.59×10^3
$\text{Hg(SO}_4)_2^{-2}$	χ_{101}	2	5	64.13×10^3	200.59×10^3
HgA_2^0	χ_{102}	0	-	355.00×10^3	200.59×10^3
Hg^{+2}	χ_{103}	2	5	-	200.59×10^3
SeO_3^{2-}	χ_{104}	2	4.5	78.96×10^3	-
HSeO_3^-	χ_{105}	1	-	78.96×10^3	-
H_2SeO_3^0	χ_{106}	0	-	78.96×10^3	-
$\text{H}_2(\text{SeO}_3)_2^{-2}$	χ_{107}	2	4.5	157.92×10^3	-

Species	(χ_i)	Z_i	\bar{a}_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
$H(SeO_3)_2^{3-}$	χ_{108}	3	4	157.92×10^3	
$Hg(SeO_3)_2^{2-}$	χ_{109}	2	4.5	157.92×10^3	200.59×10^3
$Cd(SeO_3)_2^{2-}$	χ_{110}	2	4.5	157.92×10^3	112.40×10^3
Mn_2OH^{3+}	χ_{111}	3	5	-	109.88×10^3
$Mn_2(OH)_3^+$	χ_{112}	1	6	-	109.88×10^3
$MnHCO_3^+$	χ_{113}	1	4	12.01115×10^3	54.938×10^3
$MnSO_4^0$	χ_{114}	0	-	32.06×10^3	54.938×10^3
$MnOH^+$	χ_{115}	1	4	-	54.938×10^3
$Mn(OH)_4^{-2}$	χ_{116}	2	4.5	-	54.938×10^3
$MnCl^+$	χ_{117}	1	4	35.453×10^3	54.938×10^3
$MnAc^+$	χ_{118}	1	4	24.022×10^3	54.938×10^3
$Mn(NH_3)^{+2}$	χ_{119}	2	4.5	14.0067×10^3	54.938×10^3
$Mn(NH)_2^{+2}$	χ_{120}	2	4.5	28.0134×10^3	54.938×10^3
$Mn(NH)_3^{+2}$	χ_{121}	2	4.5	42.0201×10^3	54.938×10^3
$ZnOH$	χ_{122}	1	4	-	65.38×10^3
$Zn(OH)_2^0$	χ_{123}	0	-	-	65.38×10^3
$Zn(OH)_3^-$	χ_{124}	1	4	-	65.38×10^3
$(Zn)_2OH^{+3}$	χ_{125}	3	5	-	130.76×10^3
$ZnHPO_4^0$	χ_{126}	0	-	30.9738×10^3	65.38×10^3
$ZnH_2PO_4^+$	χ_{127}	1	4.5	30.9738×10^3	65.38×10^3
$ZnSO_4^0$	χ_{128}	0	-	32.064×10^3	65.38×10^3
$Zn(SO)_2^{-2}$	χ_{129}	2	4.5	64.128×10^3	65.38×10^3
$Zn(SO_4)_3^{-4}$	χ_{130}	4	5	96.192×10^3	65.38×10^3
$ZnCl^+$	χ_{131}	1	4	35.453×10^3	65.38×10^3
$Zn(Cl)_2^0$	χ_{132}	0	-	70.906×10^3	65.38×10^3
$Zn(Cl)_3^-$	χ_{133}	1	4	106.359×10^3	65.38×10^3
$ZnAc^+$	χ_{134}	1	4	24.022×10^3	65.38×10^3
$Zn(Ac)_2^0$	χ_{135}	0	-	48.044×10^3	65.38×10^3
$Zn(Ac)_3^-$	χ_{136}	1	4.5	72.066×10^3	65.38×10^3
$Zn(NH_3)^{+2}$	χ_{137}	2	4.5	14.0067×10^3	65.38×10^3
$Zn(NH_3)_2^{+2}$	χ_{138}	2	4.5	28.0134×10^3	65.38×10^3
$Zn(NH_3)_3^{+2}$	χ_{139}	2	4.5	42.0201×10^3	65.38×10^3
$Zn(HS)(OH)^0$	χ_{140}	0	-	32.06×10^3	65.38×10^3
$NaOH^0$	χ_{141}	0	-	-	22.99×10^3
$NaHPO_4^-$	χ_{142}	1	4.5	30.9738×10^3	22.99×10^3
$NaSO_4^-$	χ_{143}	1	4.5	32.06×10^3	22.99×10^3

Species	(χ_i)	Z_i	Å_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
NaAc ⁰	χ_{144}	0	-	24.022 x 10 ³	22.99 x 10 ³
KOH ⁰	χ_{145}	0	-	-	39.098 x 10 ³
KHPO ₄ ⁻	χ_{146}	1	4.5	30.9738 x 10 ³	39.098 x 10 ³
KSO ₄ ⁻	χ_{147}	1	4.5	32.06 x 10 ³	39.098 x 10 ³
KCl ⁰	χ_{148}	0	-	35.453 x 10 ³	39.098 x 10 ³
(Hg ₂)OH ⁺	χ_{149}	1	4.5	-	200.59 x 10 ³
(Hg ₂)SO ₄ ⁰	χ_{150}	0	-	32.06 x 10 ³	200.59 x 10 ³
(Hg ₂)(SO ₄) ₄ ⁻²	χ_{151}	2	5	64.12 x 10 ³	200.59 x 10 ³
FeOH ²⁺	χ_{152}	2	6	-	55.847 x 10 ³
Fe(OH) ₂ ⁺	χ_{153}	1	4.5	-	55.847 x 10 ³
(Fe) ₂ (OH) ₂ ⁺⁴	χ_{154}	4	6	-	111.694 x 10 ³
(Fe) ₃ (OH) ₄ ⁺	χ_{155}	1	4.5	-	167.541 x 10 ³
FeHPO ₄ ⁺	χ_{156}	1	4.5	30.9738 x 10 ³	55.847 x 10 ³
FeH ₂ PO ₄ ⁺²	χ_{157}	2	5	30.9738 x 10 ³	55.847 x 10 ³
FeSO ₄ ⁺	χ_{158}	1	4.5	32.064 x 10 ³	55.847 x 10 ³
Fe(SO ₄) ₂ ⁻	χ_{159}	1	4.5	64.128 x 10 ³	55.847 x 10 ³
FeCl ⁺²	χ_{160}	2	6	35.453 x 10 ³	55.847 x 10 ³
Fe(Cl) ₂ ⁺	χ_{161}	1	4.5	70.906 x 10 ³	55.847 x 10 ³
Fe(Cl) ₃ ⁰	χ_{162}	0	-	106.359 x 10 ³	55.847 x 10 ³
FeAc ⁺²	χ_{163}	2	5	24.022 x 10 ³	55.847 x 10 ³
Fe(Ac) ₂ ⁺	χ_{164}	1	4.5	48.044 x 10 ³	55.847 x 10 ³
Fe(Ac) ₃ ⁰	χ_{165}	0	-	72.066 x 10 ³	55.847 x 10 ³
FeHSeO ₃ ⁺²	χ_{166}	2	5	78.96 x 10 ³	55.847 x 10 ³
FeHSiO ₄ ⁰	χ_{167}	0	-	28.086 x 10 ³	55.847 x 10 ³
H ₂ SiO ₄ ⁻²	χ_{168}	2	4.5	28.086 x 10 ³	-
HSiO ₄ ⁻³	χ_{169}	3	6	28.086 x 10 ³	-
H ₂ (SiO ₄) ₂ ⁻⁶	χ_{170}	6	9	56.172 x 10 ³	-
H ₄ (SiO ₄) ₄ ⁻¹²	χ_{171}	12	11	112.344 x 10 ³	-
H ₆ (SiO ₄) ₄ ⁻¹⁰	χ_{172}	10	11	112.344 x 10 ³	-
MgSiO ₄ ⁻²	χ_{173}	2	4.5	28.086 x 10 ³	24.305 x 10 ³
MgHSiO ₄ ⁻	χ_{174}	1	4	28.086 x 10 ³	24.305 x 10 ³
Mg(HSiO ₄) ₂ ⁻³	χ_{175}	3	6	56.172 x 10 ³	24.305 x 10 ³
CaSiO ₄ ⁻²	χ_{176}	2	4.5	28.086 x 10 ³	40.08 x 10 ³
CaHSiO ₄ ⁻	χ_{177}	1	4	28.086 x 10 ³	40.08 x 10 ³
Ca(HSiO ₄) ₂ ⁻⁴	χ_{178}	4	9	56.172 x 10 ³	40.08 x 10 ³
Mn ⁺²	χ_{179}	2	6	-	54.938 x 10 ³

Species	(χ_i)	Z_i	a_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
Zn^{+2}	χ_{180}	2	6	-	65.38×10^3
Na^+	χ_{181}	1	4	-	22.99×10^3
K^+	χ_{182}	1	3	-	39.098×10^3
Hg^{+}	χ_{183}	1	4	-	401.18×10^3
Fe^{+3}	χ_{184}	3	9	-	55.847×10^3
H^+	χ_{185}	1	9	-	-
SiO_4^{-3}	χ_{186}	4	5	28.086×10^3	-
A^{-2}	χ_{187}	1	4.5	177.50×10^3	-
$Zn(HS)_2^0$	χ_{188}	0	-	64.13×10^3	65.38×10^3
$EDTA^{-4}$	χ_{189}	4	6	120.1115×10^3	-
$HEDTA^{-3}$	χ_{190}	3	7.5	120.1115×10^3	-
H_2EDTA^{-2}	χ_{191}	2	-0.2	120.1115×10^3	-
H_3EDTA^{-1}	χ_{192}	1	-5.1	120.1115×10^3	-
H_4EDTA^0	χ_{193}	0	-	120.1115×10^3	-
$NaEDTA^{-3}$	χ_{194}	3	0.5	120.1115×10^3	22.99×10^3
$MgEDTA^{-2}$	χ_{195}	2	-5.8	120.1115×10^3	24.312×10^3
$MgHEDTA^{-1}$	χ_{196}	1	-8.5	120.1115×10^3	24.312×10^3
$CaEDTA^{-2}$	χ_{197}	2	-5.9	120.1115×10^3	40.08×10^3
$CaHEDTA^{-1}$	χ_{198}	1	-8.5	120.1115×10^3	40.08×10^3
$FeEDTA^{-1}$	χ_{199}	1	-8.8	120.1115×10^3	55.847×10^3
$FeHEDTA^0$	χ_{200}	0	-	120.1115×10^3	55.847×10^3
$FeOHEDTA^{-2}$	χ_{201}	2	-6.8	120.1115×10^3	55.847×10^3
$Fe(OH)_2EDTA^{-3}$	χ_{202}	3	-4.1	120.1115×10^3	55.847×10^3
$(FeOHEDTA)_2^{-4}$	χ_{203}	4	1.9	240.2230×10^3	111.694×10^3
$HgEDTA^{-2}$	χ_{204}	2	-5.8	120.1115×10^3	200.59×10^3
$HgHEDTA^{-1}$	χ_{205}	1	-8.5	120.1115×10^3	200.59×10^3
$HgOHEDTA^{-3}$	χ_{206}	3	-2.5	120.1115×10^3	200.59×10^3
$CdEDTA^{-2}$	χ_{207}	2	-5.9	120.1115×10^3	112.40×10^3
$CdHEDTA^{-1}$	χ_{208}	1	-8.5	120.1115×10^3	112.40×10^3
$CuEDTA^{-2}$	χ_{209}	2	-5.9	120.1115×10^3	63.54×10^3
$CuHEDTA^{-1}$	χ_{210}	1	-8.5	120.1115×10^3	63.54×10^3
$CuOHEDTA^{-3}$	χ_{211}	3	-0.1	120.1115×10^3	63.54×10^3
$FeEDTA^{-2}$	χ_{212}	2	-5.9	120.1115×10^3	55.847×10^3
$FeHEDTA^{-1}$	χ_{213}	1	-8.5	120.1115×10^3	55.847×10^3
$FeOHEDTA^{-3}$	χ_{214}	3	-2.5	120.1115×10^3	55.847×10^3
$Fe(OH)_2EDTA^{-4}$	χ_{215}	4	-4.1	120.1115×10^3	55.847×10^3

Species	(χ_i)	Z_i	\bar{a}_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
MnEDTA ⁻²	χ_{216}	2	-5.9	120.1115×10^3	54.938×10^3
MnHEDTA ⁻¹	χ_{217}	1	-8.5	120.1115×10^3	54.938×10^3
ZnEDTA ⁻²	χ_{218}	2	-5.9	120.1115×10^3	65.38×10^3
ZnHEDTA ⁻¹	χ_{219}	1	-8.5	120.1115×10^3	65.38×10^3
ZnOHEDTA ⁻³	χ_{220}	3	-0.1	120.1115×10^3	65.38×10^3
KEDTA ⁻³	χ_{221}	3	0.4	120.1115×10^3	39.098×10^3
Co ⁺²	χ_{222}	2	6	120.1115×10^3	58.933×10^3
CoHEDTA ⁻¹	χ_{223}	1	-8.5	120.1115×10^3	58.933×10^3
CoEDTA ⁻²	χ_{224}	2	-5.9	120.1115×10^3	58.933×10^3
CoOH ⁺	χ_{225}	1	4	-	58.933×10^3
Co(OH) ₂ ⁰	χ_{226}	0	-	-	58.933×10^3
Co(OH) ₃ ⁻¹	χ_{227}	1	4	-	58.933×10^3
Co(OH) ₄ ⁻²	χ_{228}	2	4.5	-	58.933×10^3
Co ₂ OH ⁺³	χ_{229}	3	6	-	117.8660×10^3
CoSO ₄ ⁰	χ_{230}	0	-	32.064×10^3	58.933×10^3
CoNH ₃ ⁺²	χ_{231}	2	4.5	14.0067×10^3	58.933×10^3
Co(NH ₃) ₂ ⁺²	χ_{232}	2	4.5	28.0134×10^3	58.933×10^3
Co(NH ₃) ₃ ⁺²	χ_{233}	2	4.5	42.0201×10^3	58.933×10^3
CoHPO ₄ ⁰	χ_{234}	0	-	30.978×10^3	58.933×10^3
CoAc ⁺¹	χ_{235}	1	4	24.022×10^3	58.933×10^3
NTA ⁻³	χ_{236}	3	0.8	72.0669×10^3	-
HNTA ⁻²	χ_{237}	2	0.8	72.0669×10^3	-
H ₂ NTA ⁻¹	χ_{238}	1	2.3	72.0669×10^3	-
H ₃ NTA ⁰	χ_{239}	0	-	72.0669×10^3	-
NaNTA ⁻²	χ_{240}	2	10.75	72.0669×10^3	22.99×10^3
MgNTA ⁻¹	χ_{241}	1	-6.75	72.0669×10^3	24.312×10^3
CaNTA ⁻¹	χ_{242}	1	-6.65	72.0669×10^3	40.08×10^3
Ca(NTA) ₂ ⁻⁴	χ_{243}	4	32.9	144.1338×10^3	40.08×10^3
FeNTA ⁰	χ_{244}	0	-	72.0669×10^3	55.847×10^3
Fe(NTA) ₂ ⁻³	χ_{245}	3	5.6	144.1338×10^3	55.847×10^3
FeOHNTA ⁻¹	χ_{246}	1	-8.3	72.0669×10^3	55.847×10^3
Fe(OH) ₂ NTA ⁻²	χ_{247}	2	-7.0	72.0669×10^3	55.847×10^3
HgNTA ⁻¹	χ_{248}	1	-7.1	72.0669×10^3	200.59×10^3
CdNTA ⁻¹	χ_{249}	1	-7.5	72.0669×10^3	112.40×10^3
Cd(NTA) ₂ ⁻⁴	χ_{250}	4	32.9	144.1338×10^3	112.40×10^3
CdOHNTA ⁻²	χ_{251}	2	-6.3	72.0669×10^3	112.40×10^3

Species	(χ_i)	Z_i	a_i (25°C)	Anion Conversion Factor	Cation Conversion Factor
CuNTA ⁻¹	χ_{252}	1	-7.0	72.0669×10^3	63.54×10^3
Cu(NTA) ₂ ⁻⁴	χ_{253}	4	32.9	144.1338×10^3	63.54×10^3
CuOHNTA ⁻²	χ_{254}	2	-6.07	72.0669×10^3	63.54×10^3
FeNTA ⁻¹	χ_{255}	1	-7.0	72.0669×10^3	55.847×10^3
Fe(NTA) ₂ ⁻⁴	χ_{256}	4	32.9	144.1338×10^3	55.847×10^3
FeHNTA ⁰	χ_{257}	0	-	72.0669×10^3	55.847×10^3
FeOHNTA ⁻²	χ_{258}	2	-6.07	72.0669×10^3	55.847×10^3
MnNTA ⁻¹	χ_{259}	1	-7.0	72.0669×10^3	54.938×10^3
Mn(NTA) ₂ ⁻⁴	χ_{260}	4	32.9	144.1338×10^3	54.938×10^3
ZnNTA ⁻¹	χ_{261}	1	-7.0	72.0669×10^3	65.38×10^3
Zn(NTA) ₂ ⁻⁴	χ_{262}	4	32.9	144.1338×10^3	65.38×10^3
ZnOHNTA ⁻²	χ_{263}	2	-6.07	72.0669×10^3	65.38×10^3
CoNTA ⁻¹	χ_{264}	1	-7.0	72.0669×10^3	58.933×10^3
Co(NTA) ₂ ⁻⁴	χ_{265}	4	32.9	144.1338×10^3	58.933×10^3
CoOHNTA ⁻²	χ_{266}	2	-6.07	72.0669×10^3	58.933×10^3
NaOH	χ_{267}	0	-	-	22.990×10^3
H ₃ SiO ₄ ⁻	χ_{268}	1	4	28.086×10^3	-
H ₄ SiO ₄ ⁰	χ_{269}	0	-	28.086×10^3	-
C(SS)	χ_{270}	0	-	-	-
Cd(SS)	χ_{271}	0	-	-	-
Cu(SS)	χ_{272}	0	-	-	-
Fe _(II) (SS)	χ_{273}	0	-	-	-
Fe _(III) (SS)	χ_{274}	0	-	-	-
Mn(SS)	χ_{275}	0	-	-	-
Zn(SS)	χ_{276}	0	-	-	-
K(SS)	χ_{277}	0	-	-	-
Co(SS)	χ_{278}	0	-	-	-
Na(SS)	χ_{279}	0	-	-	-
Mg(SS)	χ_{280}	0	-	-	-
Ca(SS)	χ_{281}	0	-	-	-
Hg _(I) (SS)	χ_{282}	0	-	-	-
Hg _(II) (SS)	χ_{283}	0	-	-	-
Al ⁺³	χ_{284}	3	9	-	26.982×10^3
AlOH ⁺²	χ_{285}	2	6	-	26.982×10^3
Al(OH) ₂ ⁺	χ_{286}	1	4.5	-	26.982×10^3
Al(OH) ₃ ⁰	χ_{287}	0	-	-	26.982×10^3

Species	(χ_i)	Z_i	$\bar{a}_i (25^\circ C)$	Anion Conversion Factor	Cation Conversion Factor
Al(OH)_4^-	χ_{288}	1	5	-	26.982×10^3
$\text{Al}_2(\text{OH})_2^{+4}$	χ_{289}	4	6	-	26.982×10^3
$\text{Al}_3(\text{OH})_4^{+5}$	χ_{290}	1	8.8	-	26.982×10^3
AlEDTA^-	χ_{291}	0	-	120.1115×10^3	26.982×10^3
AlHEDTA^0	χ_{292}	2	6.8	120.1115×10^3	26.982×10^3
AlOHEDTA^{-2}	χ_{293}	0	-	120.1115×10^3	26.982×10^3
AlNTA^0	χ_{294}	0	-	72.0669×10^3	26.982×10^3
AlHNTA^+	χ_{295}	1	8.3	72.0669×10^3	26.982×10^3
AlOHNTA^-	χ_{296}	2	7	72.0669×10^3	26.982×10^3
$\text{Al}(\text{OH})_2\text{NTA}^{-2}$	χ_{297}	2	7	72.0669×10^3	26.982×10^3
AlA_C^{+2}	χ_{298}	2	5	24.022×10^3	26.982×10^3
AlCO_3^+	χ_{299}	1	4.5	12.01115×10^3	26.982×10^3
AlSO_4^+	χ_{300}	1	-	32.064×10^3	26.982×10^3
$\text{Al}(\text{SO}_4)_2^-$	χ_{301}	1	4.5	64.128×10^3	26.982×10^3
$\text{AlH}_2\text{PO}_4^{+2}$	χ_{302}	2	5.0	30.9738×10^3	26.982×10^3
$\text{Al}(\text{H}_2\text{PO}_4)_2^+$	χ_{303}	1	5.5	61.9476×10^3	26.982×10^3
$\text{Al}(\text{H}_2\text{PO}_4)_3^0$	χ_{304}	0	-	92.9214×10^3	26.982×10^3
AlA_2^0	χ_{305}	0	-	355.00×10^3	26.982×10^3
F^-	χ_{306}	1	3.5	18.9984×10^3	-
HF^0	χ_{307}	0	0	18.9984×10^3	-
AlF^{+2}	χ_{308}	2	6	18.9984×10^3	26.982×10^3
AlF_2^+	χ_{309}	1	4.5	37.9968×10^3	26.982×10^3
AlF_3^0	χ_{310}	0	0	56.9952×10^3	26.982×10^3
AlF_4^-	χ_{311}	1	4	75.9936×10^3	26.982×10^3
MgF^+	χ_{312}	1	4	18.9984×10^3	24.312×10^3
CaF^+	χ_{313}	1	4	18.9984×10^3	40.08×10^3
CuF^+	χ_{314}	1	4	18.9984×10^3	63.54×10^3
HgF^+	χ_{315}	1	4.5	18.9984×10^3	200.59×10^3
ZnF^+	χ_{316}	1	4	18.9984×10^3	65.38×10^3
FeF^{+2}	χ_{317}	2	6	18.9984×10^3	55.847×10^3
FeF_2^+	χ_{318}	1	4.5	37.9968×10^3	55.847×10^3
FeF_3^0	χ_{319}	0	0	56.9952×10^3	55.847×10^3

 Appendix 3. Indexed γ 's defining α 's.

$$\alpha_1 = \frac{\gamma_2}{\gamma_4}$$

$$\alpha_{10} = \frac{\gamma_5 \gamma_6}{\gamma_{10}}$$

$$\alpha_2 = \frac{\gamma_1}{\gamma_2}$$

$$\alpha_{11} = \gamma_4$$

$$\alpha_3 = \frac{\gamma_3 \gamma_6}{\gamma_8}$$

$$\alpha_{12} = 1$$

$$\alpha_4 = \frac{\gamma_3 \gamma_1}{\gamma_7}$$

$$\alpha_{13} = \frac{\gamma_3 \gamma_{17}}{\gamma_{13}}$$

$$\alpha_5 = \frac{\gamma_5 \gamma_1}{\gamma_9}$$

$$\alpha_{14} = \frac{\gamma_5 \gamma_{17}}{\gamma_{14}}$$

$$\alpha_6 = \gamma_3 \gamma_1$$

$$\alpha_{15} = \frac{\gamma_{15}}{\gamma_6}$$

$$\alpha_7 = \gamma_5 \gamma_3 \gamma_1^2$$

$$\alpha_{16} = \frac{1}{\gamma_{15}}$$

$$\alpha_8 = \frac{\gamma_3 \gamma_2}{\gamma_{11}}$$

$$\alpha_{17} = \gamma_{17}$$

$$\alpha_9 = \frac{\gamma_5 \gamma_2}{\gamma_{12}}$$

$$\alpha_{18} = \frac{\gamma_{19}}{\gamma_{18} \gamma_1}$$

Appendix 3. (cont'd).

$$\alpha_{19} = \frac{\gamma_{20}}{\gamma_{18} \gamma_1^2}$$

$$\alpha_{27} = \frac{\gamma_{27}}{\gamma_{18} \gamma_1}$$

$$\alpha_{20} = \gamma_{18}$$

$$\alpha_{28} = \frac{\gamma_{28}}{\gamma_{18} \gamma_{16}}$$

$$\alpha_{21} = \frac{\gamma_{21}}{\gamma_{18}}$$

$$\alpha_{29} = \frac{\gamma_{29}}{\gamma_{18} \gamma_{16}^2}$$

$$\alpha_{22} = \frac{\gamma_{22}}{\gamma_{18}}$$

$$\alpha_{30} = \gamma_{18} \gamma_{17}^2$$

$$\alpha_{23} = \frac{\gamma_{23}}{\gamma_{18}}$$

$$\alpha_{31} = \frac{\gamma_{31}}{\gamma_{18} \gamma_{35}}$$

$$\alpha_{24} = \frac{\gamma_{24}}{\gamma_{18}}$$

$$\alpha_{32} = \frac{\gamma_{32}}{\gamma_{18} \gamma_{35}^2}$$

$$\alpha_{25} = \frac{\gamma_{25}}{\gamma_{18}^2}$$

$$\alpha_{33} = \frac{\gamma_{33}}{\gamma_{18} \gamma_{35}^3}$$

$$\alpha_{26} = \frac{\gamma_{26}}{\gamma_6 \gamma_{18}}$$

$$\alpha_{34} = 1$$

Appendix 3. (cont'd).

$$\alpha_{35} = \frac{\gamma_{35}}{\gamma_{34}}$$

$$\alpha_{44} = \frac{\gamma_{44}}{\gamma_{40}}$$

$$\alpha_{36} = \frac{\gamma_{36}}{\gamma_{18} \gamma_{38}}$$

$$\alpha_{45} = \frac{\gamma_{45}}{\gamma_{40}^2}$$

$$\alpha_{37} = \frac{\gamma_{37}}{\gamma_{18} \gamma_{38}}$$

$$\alpha_{46} = \frac{\gamma_{46}}{\gamma_{40} \gamma_6}$$

$$\alpha_{38} = \frac{\gamma_{39}}{\gamma_{38}}$$

$$\alpha_{39} = \gamma_{18} \gamma_1$$

$$\alpha_{47} = \frac{\gamma_{47}}{\gamma_{40} \gamma_{16}}$$

$$\alpha_{40} = \gamma_{40} \gamma_{17}^2$$

$$\alpha_{48} = \frac{\gamma_{48}}{\gamma_{40} \gamma_{16}^2}$$

$$\alpha_{41} = \frac{\gamma_{41}}{\gamma_{40}}$$

$$\alpha_{49} = \frac{\gamma_{49}}{\gamma_{40} \gamma_{16}^3}$$

$$\alpha_{42} = \frac{\gamma_{42}}{\gamma_{40}}$$

$$\alpha_{50} = \frac{\gamma_{50}}{\gamma_{40} \gamma_{35}}$$

$$\alpha_{43} = \frac{\gamma_{43}}{\gamma_{40}}$$

$$\alpha_{51} = \frac{\gamma_{51}}{\gamma_{40} \gamma_{35}^2}$$

Appendix 3. (cont'd).

$$\alpha_{52} = \frac{\gamma_{52}}{\gamma_{40} \gamma_{35}^3}$$

$$\alpha_{60} = \frac{\gamma_{60}}{\gamma_{61}}$$

$$\alpha_{53} = \frac{\gamma_{53}}{\gamma_{54}}$$

$$\alpha_{61} = \gamma_{61} \gamma_{40}$$

$$\alpha_{54} = \frac{\gamma_{54}}{\gamma_{55}}$$

$$\alpha_{63} = \gamma_{18} \gamma_{61}$$

$$\alpha_{55} = \frac{\gamma_{55}}{\gamma_{62}}$$

$$\alpha_{64} = \gamma_{18}^2 \gamma_{61}$$

$$\alpha_{56} = \frac{\gamma_{56}}{\gamma_{40} \gamma_{38}}$$

$$\alpha_{65} = \gamma_{18}^2 \gamma_{17}^2 \gamma_1$$

$$\alpha_{57} = \frac{\gamma_{57}}{\gamma_{40} \gamma_{38}^2}$$

$$\alpha_{66} = \gamma_{18}^3 \gamma_{17}^2 \gamma_1^2$$

$$\alpha_{58} = \frac{\gamma_{58}}{\gamma_{40} \gamma_{38}^3}$$

$$\alpha_{68} = \gamma_{40}^3 \gamma_{62}^2$$

$$\alpha_{59} = \frac{\gamma_{59}}{\gamma_{60}}$$

$$\alpha_{69} = \gamma_{18}^4 \gamma_6 \gamma_{17}^6$$

Appendix 3. (cont'd).

$$\alpha_{70} = \gamma^2_{18} \gamma_{16} \gamma^3_{17}$$

$$\alpha_{78} = \gamma^4_3 \gamma^3_{62}$$

$$\alpha_{71} = 1$$

$$\alpha_{79} = \frac{\gamma_{67}}{\gamma_5 \gamma_{62}}$$

$$\alpha_{72} = \frac{\gamma_{64}}{\gamma_3 \gamma_{62}}$$

$$\alpha_{80} = \frac{\gamma_{68}}{\gamma_5 \gamma_{55}}$$

$$\alpha_{73} = \frac{\gamma_{65}}{\gamma_3 \gamma_{55}}$$

$$\alpha_{81} = \frac{\gamma_{69}}{\gamma_5 \gamma_{54}}$$

$$\alpha_{74} = \frac{\gamma_{66}}{\gamma_3 \gamma_{54}}$$

$$\alpha_{82} = \gamma^5_5 \gamma^3_{62} \gamma_{17}$$

$$\alpha_{75} = \gamma^5_3 \gamma^3_{62} \gamma_{17}$$

$$\alpha_{83} = \gamma_5 \gamma_{55}$$

$$\alpha_{76} = \gamma_3 \gamma_{55}$$

$$\alpha_{84} = \gamma^3_5 \gamma^2_{62}$$

$$\alpha_{77} = \gamma^3_3 \gamma^2_{62}$$

$$\alpha_{85} = \gamma^4_5 \gamma^3_{62}$$

$$\alpha_{86} = \frac{\gamma_{73}}{\gamma_{72}}$$

 Appendix 3. (cont'd).

$$\alpha_{87} = \frac{\gamma_{74}}{\gamma_{72}}$$

$$\alpha_{95} = \gamma_{72} \gamma_{17}^2$$

$$\alpha_{88} = \frac{\gamma_{75}}{\gamma_{72}}$$

$$\alpha_{96} = \gamma_{72}^3 \gamma_{62}^2$$

$$\alpha_{97} = \gamma_{72} \gamma_1$$

$$\alpha_{89} = \frac{\gamma_{76}}{\gamma_{72} \gamma_{17}^4}$$

$$\alpha_{98} = \frac{\gamma_{81}}{\gamma_{40} \gamma_{60}}$$

$$\alpha_{90} = \frac{\gamma_{80}}{\gamma_{72} \gamma_6}$$

$$\alpha_{99} = \frac{\gamma_{82}}{\gamma_{40} \gamma_{60}^2}$$

$$\alpha_{91} = \frac{\gamma_{77}}{\gamma_{72} \gamma_{55}}$$

$$\alpha_{100} = \frac{\gamma_{83}}{\gamma_{40} \gamma_{60}^3}$$

$$\alpha_{92} = \frac{\gamma_{78}}{\gamma_{72} \gamma_{54}}$$

$$\alpha_{101} = \frac{\gamma_{84}}{\gamma_{103} \gamma_{17}}$$

$$\alpha_{93} = \frac{\gamma_{79}}{\gamma_{72} \gamma_{38}}$$

$$\alpha_{102} = \frac{\gamma_{85}}{\gamma_{103} \gamma_{17}^2}$$

$$\alpha_{94} = \gamma_{72} \gamma_{61}$$

 Appendix 3. (cont'd).

$$\alpha_{103} = \frac{\gamma_{86}}{\gamma_{103} \gamma_{17}^3}$$

$$\alpha_{111} = \frac{\gamma_{94}}{\gamma_{103} \gamma_{35}^2}$$

$$\alpha_{104} = \frac{\gamma_{87}}{\gamma_{103}^2 \gamma_{17}}$$

$$\alpha_{112} = \frac{\gamma_{95}}{\gamma_{103} \gamma_{35}^3}$$

$$\alpha_{105} = \frac{\gamma_{88}}{\gamma_{103}^3 \gamma_{17}^3}$$

$$\alpha_{113} = \frac{\gamma_{96}}{\gamma_{103} \gamma_{38}}$$

$$\alpha_{106} = \frac{\gamma_{89}}{\gamma_{103} \gamma_{17} \gamma_{16}}$$

$$\alpha_{114} = \frac{\gamma_{97}}{\gamma_{103} \gamma_{38}^2}$$

$$\alpha_{107} = \frac{\gamma_{90}}{\gamma_{103} \gamma_{16}}$$

$$\alpha_{115} = \frac{\gamma_{98}}{\gamma_{103} \gamma_{38}^3}$$

$$\alpha_{109} = \frac{\gamma_{92}}{\gamma_{103} \gamma_{16}^3}$$

$$\alpha_{116} = \frac{\gamma_{99}}{\gamma_{103} \gamma_{60}^2}$$

$$\alpha_{110} = \frac{\gamma_{93}}{\gamma_{103} \gamma_{35}}$$

$$\alpha_{117} = \frac{\gamma_{100}}{\gamma_{103} \gamma_6}$$

Appendix 3. (cont'd).

$$\alpha_{118} = \frac{\gamma_{101}}{\gamma_{103} \gamma_6^2}$$

$$\alpha_{126} = \frac{\gamma_{107}}{\gamma_{108}}$$

$$\alpha_{119} = \frac{\gamma_{102}}{\gamma_{103} \gamma_{71}^2}$$

$$\alpha_{127} = \frac{\gamma_{109}}{\gamma_{103} \gamma_{104}}$$

$$\alpha_{120} = \gamma_{103} \gamma_{17}^2$$

$$\alpha_{128} = \frac{\gamma_{110}}{\gamma_{40} \gamma_{104}^2}$$

$$\alpha_{121} = \gamma_{103} \gamma_{61}$$

$$\alpha_{129} = \gamma_{103} \gamma_{104}$$

$$\alpha_{122} = \gamma_{103} \gamma_{61}$$

$$\alpha_{130} = \gamma_{18} \gamma_{104}$$

$$\alpha_{123} = \frac{\gamma_{105}}{\gamma_{104}}$$

$$\alpha_{131} = \gamma_5 \gamma_{104}$$

$$\alpha_{124} = \frac{1}{\gamma_{105}}$$

$$\alpha_{132} = \frac{\gamma_{115}}{\gamma_{179} \gamma_{17}}$$

$$\alpha_{125} = \frac{\gamma_{107}}{\gamma_{105}^2}$$

$$\alpha_{133} = \frac{\gamma_{116}}{\gamma_{179} \gamma_{17}^4}$$

Appendix 3. (cont'd).

$$\alpha_{134} = \frac{\gamma_{111}}{\gamma_{179}^2 \gamma_{17}}$$

$$\alpha_{142} = \frac{\gamma_{121}}{\gamma_{179} \gamma_{35}^3}$$

$$\alpha_{135} = \frac{\gamma_{112}}{\gamma_{179}^2 \gamma_{17}^3}$$

$$\alpha_{143} = \frac{\gamma_{122}}{\gamma_{180} \gamma_{17}}$$

$$\alpha_{136} = \frac{\gamma_{113}}{\gamma_{179} \gamma_2}$$

$$\alpha_{144} = \frac{\gamma_{123}}{\gamma_{180} \gamma_{17}^2}$$

$$\alpha_{137} = \frac{\gamma_{114}}{\gamma_{179} \gamma_6}$$

$$\alpha_{145} = \frac{\gamma_{124}}{\gamma_{180} \gamma_{17}^3}$$

$$\alpha_{138} = \frac{\gamma_{117}}{\gamma_{179} \gamma_{16}}$$

$$\alpha_{146} = \frac{\gamma_{125}}{\gamma_{180}^2 \gamma_{17}}$$

$$\alpha_{139} = \frac{\gamma_{118}}{\gamma_{179} \gamma_{38}}$$

$$\alpha_{147} = \frac{\gamma_{126}}{\gamma_{180} \gamma_{55}}$$

$$\alpha_{140} = \frac{\gamma_{119}}{\gamma_{179} \gamma_{35}}$$

$$\alpha_{141} = \frac{\gamma_{120}}{\gamma_{179}^2 \gamma_{35}^2}$$

$$\alpha_{148} = \frac{\gamma_{127}}{\gamma_{180} \gamma_{54}}$$

Appendix 3. (cont'd).

$$\alpha_{149} = \frac{\gamma_{128}}{\gamma_{180} \gamma_6}$$

$$\alpha_{155} = \frac{\gamma_{134}}{\gamma_{180} \gamma_{38}}$$

$$\alpha_{150} = \frac{\gamma_{129}}{\gamma_{180} \gamma_6^2}$$

$$\alpha_{156} = \frac{\gamma_{135}}{\gamma_{180} \gamma_{38}^2}$$

$$\alpha_{151} = \frac{\gamma_{130}}{\gamma_{180} \gamma_6^3}$$

$$\alpha_{157} = \frac{\gamma_{136}}{\gamma_{180} \gamma_{38}^3}$$

$$\alpha_{152} = \frac{\gamma_{131}}{\gamma_{180} \gamma_{16}}$$

$$\alpha_{158} = \frac{\gamma_{137}}{\gamma_{180} \gamma_{35}}$$

$$\alpha_{153} = \frac{\gamma_{132}}{\gamma_{180} \gamma_{16}^2}$$

$$\alpha_{159} = \frac{\gamma_{138}}{\gamma_{180} \gamma_{35}^2}$$

$$\alpha_{154} = \frac{\gamma_{133}}{\gamma_{180} \gamma_{16}^3}$$

$$\alpha_{160} = \frac{\gamma_{139}}{\gamma_{180} \gamma_{35}^3}$$

Appendix 3. (cont'd).

$$\alpha_{161} = \frac{\gamma_{140}}{\gamma_{180} \gamma_{17} \gamma_{60}}$$

$$\alpha_{169} = \frac{\gamma_{148}}{\gamma_{182} \gamma_{16}}$$

$$\alpha_{162} = \frac{\gamma_{141}}{\gamma_{181} \gamma_{17}}$$

$$\alpha_{170} = \frac{\gamma_{149}}{\gamma_{183} \gamma_{17}}$$

$$\alpha_{163} = \frac{\gamma_{142}}{\gamma_{181} \gamma_{55}}$$

$$\alpha_{171} = \frac{\gamma_{150}}{\gamma_{183} \gamma_6}$$

$$\alpha_{164} = \frac{\gamma_{143}}{\gamma_{181} \gamma_6}$$

$$\alpha_{172} = \frac{\gamma_{151}}{\gamma_{183}^2 \gamma_6^2}$$

$$\alpha_{165} = \frac{\gamma_{144}}{\gamma_{181} \gamma_{38}}$$

$$\alpha_{173} = \frac{\gamma_{152}}{\gamma_{184} \gamma_{17}}$$

$$\alpha_{166} = \frac{\gamma_{145}}{\gamma_{182} \gamma_{17}}$$

$$\alpha_{174} = \frac{\gamma_{153}}{\gamma_{184}^2 \gamma_{17}^2}$$

$$\alpha_{167} = \frac{\gamma_{146}}{\gamma_{182} \gamma_{55}}$$

$$\alpha_{175} = \frac{\gamma_{154}}{\gamma_{184}^2 \gamma_{17}^2}$$

$$\alpha_{168} = \frac{\gamma_{147}}{\gamma_{182} \gamma_6}$$

$$\alpha_{176} = \frac{\gamma_{155}}{\gamma_{184}^3 \gamma_{17}^4}$$

 Appendix 3. (cont'd).

$$\alpha_{177} = \frac{\gamma_{156}}{\gamma_{184} \gamma_{55}}$$

$$\alpha_{185} = \frac{\gamma_{164}}{\gamma_{184} \gamma_{38}^2}$$

$$\alpha_{178} = \frac{\gamma_{157}}{\gamma_{184} \gamma_{54}}$$

$$\alpha_{186} = \frac{\gamma_{165}}{\gamma_{184} \gamma_{38}^3}$$

$$\alpha_{179} = \frac{\gamma_{158}}{\gamma_{184} \gamma_6}$$

$$\alpha_{187} = \frac{\gamma_{166}}{\gamma_{184} \gamma_{105}}$$

$$\alpha_{180} = \frac{\gamma_{159}}{\gamma_{184} \gamma_6^2}$$

$$\alpha_{188} = \frac{\gamma_{167}}{\gamma_{169} \gamma_{184}}$$

$$\alpha_{181} = \frac{\gamma_{160}}{\gamma_{184} \gamma_{16}}$$

$$\alpha_{189} = \frac{\gamma_{168}}{\gamma_{169}}$$

$$\alpha_{182} = \frac{\gamma_{161}}{\gamma_{184} \gamma_{16}^2}$$

$$\alpha_{190} = \frac{\gamma_{169}}{\gamma_{186}}$$

$$\alpha_{183} = \frac{\gamma_{162}}{\gamma_{184} \gamma_{16}^3}$$

$$\alpha_{191} = \frac{\gamma_{170}}{\gamma_{186}^2}$$

$$\alpha_{184} = \frac{\gamma_{163}}{\gamma_{184} \gamma_{38}}$$

$$\alpha_{192} = \frac{\gamma_{171}}{\gamma_{186}^4}$$

Appendix 3. (cont'd).

$$\alpha_{193} = \frac{\gamma_{172}}{\gamma_5^4 \gamma_{186}}$$

$$\alpha_{201} = \gamma_{179} \gamma_{17}^2$$

$$\alpha_{202} = \gamma_{179} \gamma_1$$

$$\alpha_{194} = \frac{\gamma_{173}}{\gamma_5 \gamma_{186}}$$

$$\alpha_{203} = \gamma_{179} \gamma_{61}$$

$$\alpha_{195} = \frac{\gamma_{174}}{\gamma_5 \gamma_{169}}$$

$$\alpha_{204} = \gamma_{179} \gamma_{61}$$

$$\alpha_{196} = \frac{\gamma_{175}}{\gamma_5 \gamma_{169}^2}$$

$$\alpha_{205} = \gamma_{179} \gamma_{104}$$

$$\alpha_{206} = \gamma_{180} \gamma_{17}^2$$

$$\alpha_{197} = \frac{\gamma_{176}}{\gamma_3 \gamma_{186}}$$

$$\alpha_{207} = \gamma_{180} \gamma_{17}$$

$$\alpha_{198} = \frac{\gamma_{177}}{\gamma_3 \gamma_{169}}$$

$$\alpha_{208} = \gamma_{180} \gamma_1$$

$$\alpha_{199} = \frac{\gamma_{178}}{\gamma_3 \gamma_{169}^2}$$

$$\alpha_{209} = \gamma_{180}^3 \gamma_{62}^2$$

$$\alpha_{210} = \gamma_{180} \gamma_{61}$$

$$\alpha_{200} = \gamma_5^2 \gamma_{169}^3$$

Appendix 3. (cont'd).

$$\alpha_{211} = \gamma_3 \gamma_{186}$$

$$\alpha_{221} = \frac{\gamma_{190}}{\gamma_{189}}$$

$$\alpha_{212} = \gamma_{183} \gamma_{16}^2$$

$$\alpha_{222} = \frac{\gamma_{191}}{\gamma_{190}}$$

$$\alpha_{213} = \gamma_{184} \gamma_{17}^3$$

$$\alpha_{223} = \frac{\gamma_{192}}{\gamma_{191}}$$

$$\alpha_{214} = \gamma_{184} \gamma_{17}^3$$

$$\alpha_{224} = \frac{1}{\gamma_{192}}$$

$$\alpha_{215} = \gamma_{184} \gamma_{17}^3$$

$$\alpha_{216} = \gamma_{183} \gamma_1$$

$$\alpha_{225} = \frac{\gamma_{193}}{\gamma_{181} \gamma_{189}}$$

$$\alpha_{217} = \gamma_{184} \gamma_{62}$$

$$\alpha_{226} = \frac{\gamma_{195}}{\gamma_5 \gamma_{189}}$$

$$\alpha_{218} = \gamma_{183} \gamma_{55}$$

$$\alpha_{227} = \frac{\gamma_{196}}{\gamma_{195}}$$

$$\alpha_{219} = \gamma_{183} \gamma_6$$

$$\alpha_{228} = \frac{\gamma_{197}}{\gamma_3 \gamma_{189}}$$

$$\alpha_{220} = \frac{1}{\gamma_{180} \gamma_{60}^2}$$

Appendix 3. (cont'd).

$$\alpha_{229} = \frac{\gamma_{198}}{\gamma_{197}}$$

$$\alpha_{237} = \frac{\gamma_{204}}{\gamma_{206}}$$

$$\alpha_{230} = \frac{\gamma_{199}}{\gamma_{184} \gamma_{189}}$$

$$\alpha_{238} = \frac{\gamma_{207}}{\gamma_{40} \gamma_{189}}$$

$$\alpha_{231} = \frac{1}{\gamma_{199}}$$

$$\alpha_{239} = \frac{\gamma_{208}}{\gamma_{207}}$$

$$\alpha_{232} = \frac{\gamma_{199}}{\gamma_{201}}$$

$$\alpha_{240} = \frac{\gamma_{209}}{\gamma_{18} \gamma_{189}}$$

$$\alpha_{233} = \frac{\gamma_{201}}{\gamma_{202}}$$

$$\alpha_{241} = \frac{\gamma_{210}}{\gamma_{209}}$$

$$\alpha_{234} = \frac{\gamma_{199}}{\gamma_{203}}$$

$$\alpha_{242} = \frac{\gamma_{211}}{\gamma_{209} \gamma_{17}}$$

$$\alpha_{235} = \frac{\gamma_{204}}{\gamma_{103} \gamma_{189}}$$

$$\alpha_{243} = \frac{\gamma_{212}}{\gamma_{72} \gamma_{189}}$$

$$\alpha_{236} = \frac{\gamma_{205}}{\gamma_{204}}$$

$$\alpha_{244} = \frac{\gamma_{213}}{\gamma_{212}}$$

Appendix 3. (cont'd).

$$\alpha_{245} = \frac{\gamma_{212}}{\gamma_{214}}$$

$$\alpha_{253} = \frac{\gamma_{224}}{\gamma_{222} \gamma_{189}}$$

$$\alpha_{246} = \frac{\gamma_{214}}{\gamma_{215}}$$

$$\alpha_{254} = \frac{\gamma_{223}}{\gamma_{224}}$$

$$\alpha_{247} = \frac{\gamma_{216}}{\gamma_{179} \gamma_{189}}$$

$$\alpha_{255} = \frac{\gamma_{225}}{\gamma_{222} \gamma_{17}}$$

$$\alpha_{248} = \frac{\gamma_{217}}{\gamma_{216}}$$

$$\alpha_{256} = \frac{1}{\gamma_{222} \gamma_{17}^2}$$

$$\alpha_{249} = \frac{\gamma_{218}}{\gamma_{180} \gamma_{189}}$$

$$\alpha_{257} = \frac{\gamma_{227}}{\gamma_{222} \gamma_{17}^3}$$

$$\alpha_{250} = \frac{\gamma_{219}}{\gamma_{218}}$$

$$\alpha_{258} = \frac{\gamma_{228}}{\gamma_{222} \gamma_{17}^4}$$

$$\alpha_{251} = \frac{\gamma_{220}}{\gamma_{218} \gamma_{17}}$$

$$\alpha_{259} = \frac{\gamma_{229}}{\gamma_{222}^2 \gamma_{17}}$$

$$\alpha_{252} = \frac{\gamma_{221}}{\gamma_{182} \gamma_{189}}$$

Appendix 3. (cont'd)

$$\alpha_{260} = \frac{1}{\gamma_{222} \gamma_6}$$

$$\alpha_{268} = \frac{\gamma_{239}}{\gamma_{238}}$$

$$\alpha_{261} = \frac{\gamma_{231}}{\gamma_{222} \gamma_{35}}$$

$$\alpha_{269} = \frac{\gamma_{241}}{\gamma_5 \gamma_{236}}$$

$$\alpha_{262} = \frac{\gamma_{232}}{\gamma_{222} \gamma_{35}^2}$$

$$\alpha_{270} = \frac{\gamma_{242}}{\gamma_3 \gamma_{236}}$$

$$\alpha_{263} = \frac{\gamma_{233}}{\gamma_{222} \gamma_{35}^3}$$

$$\alpha_{271} = \frac{\gamma_{243}}{\gamma_3 \gamma_{236}^2}$$

$$\alpha_{264} = \frac{1}{\gamma_{222} \gamma_{62}}$$

$$\alpha_{272} = \frac{\gamma_{255}}{\gamma_{72} \gamma_{236}}$$

$$\alpha_{265} = \frac{\gamma_{235}}{\gamma_{222} \gamma_{38}}$$

$$\alpha_{273} = \frac{\gamma_{256}}{\gamma_{72} \gamma_{236}^2}$$

$$\alpha_{266} = \frac{\gamma_{237}}{\gamma_{236}}$$

$$\alpha_{274} = \frac{\gamma_{257}}{\gamma_{25}}$$

$$\alpha_{267} = \frac{\gamma_{238}}{\gamma_{237}}$$

$$\alpha_{276} = \frac{\gamma_{264}}{\gamma_{224} \gamma_{236}}$$

$$\alpha_{275} = \frac{\gamma_{255}}{\gamma_{258}}$$

Appendix 3. (cont'd).

$$\alpha_{277} = \frac{\gamma_{265}}{\gamma_{222} \gamma_{236}^2}$$

$$\alpha_{285} = \frac{1}{\gamma_{246}}$$

$$\alpha_{278} = \frac{\gamma_{264}}{\gamma_{265}}$$

$$\alpha_{286} = \frac{\gamma_{246}}{\gamma_{247}}$$

$$\alpha_{279} = \frac{\gamma_{252}}{\gamma_{18} \gamma_{236}}$$

$$\alpha_{287} = \frac{\gamma_{261}}{\gamma_{180} \gamma_{236}}$$

$$\alpha_{280} = \frac{\gamma_{253}}{\gamma_{18} \gamma_{236}^2}$$

$$\alpha_{288} = \frac{\gamma_{262}}{\gamma_{180} \gamma_{236}^2}$$

$$\alpha_{281} = \frac{\gamma_{254}}{\gamma_{252}}$$

$$\alpha_{289} = \frac{\gamma_{263}}{\gamma_{261}}$$

$$\alpha_{282} = \frac{\gamma_{252}}{\gamma_{254}}$$

$$\alpha_{290} = \frac{\gamma_{261}}{\gamma_{263}}$$

$$\alpha_{283} = \frac{1}{\gamma_{184} \gamma_{236}}$$

$$\alpha_{291} = \frac{\gamma_{249}}{\gamma_{40} \gamma_{236}}$$

$$\alpha_{284} = \frac{\gamma_{245}}{\gamma_{184} \gamma_{236}^2}$$

$$\alpha_{292} = \frac{\gamma_{250}}{\gamma_{40} \gamma_{236}^2}$$

Appendix 3. (cont'd).

$$\alpha_{293} = \frac{\gamma_{249}}{\gamma_{251}}$$

$$\alpha_{301} = \gamma_{222} \gamma_{61}$$

$$\alpha_{294} = \frac{\gamma_{248}}{\gamma_{103} \gamma_{236}}$$

$$\alpha_{302} = \frac{\gamma_{269}}{\gamma_{268}}$$

$$\alpha_{295} = \frac{\gamma_{240}}{\gamma_{181} \gamma_{236}}$$

$$\alpha_{303} = \frac{\gamma_{268}}{\gamma_{168}}$$

$$\alpha_{296} = \frac{\gamma_{259}}{\gamma_{179} \gamma_{236}}$$

$$\alpha_{304} = 1$$

$$\alpha_{297} = \frac{\gamma_{260}}{\gamma_{179} \gamma_{236}^2}$$

$$\alpha_{305} = 1$$

$$\alpha_{306} = 1$$

$$\alpha_{298} = \gamma_{222} \gamma_1$$

$$\alpha_{307} = 1$$

$$\alpha_{299} = \gamma_{222} \gamma_{17}^2$$

$$\alpha_{308} = 1$$

$$\alpha_{300} = \gamma_{222} \gamma_{62}^2$$

$$\alpha_{309} = 1$$

Appendix 3. (cont'd).

$$\alpha_{310} = 1$$

$$\alpha_{319} = \frac{\gamma_{287}}{\gamma_{284}\gamma_{17}^3}$$

$$\alpha_{311} = 1$$

$$\alpha_{312} = 1$$

$$\alpha_{320} = \frac{\gamma_{288}}{\gamma_{284}\gamma_{17}^4}$$

$$\alpha_{313} = 1$$

$$\alpha_{321} = \frac{\gamma_{289}}{\gamma_{284}\gamma_{17}^2}$$

$$\alpha_{314} = 1$$

$$\alpha_{315} = 1$$

$$\alpha_{322} = \frac{\gamma_{290}}{\gamma_{284}\gamma_{17}^3}$$

$$\alpha_{316} = 1$$

$$\alpha_{323} = \frac{\gamma_{291}}{\gamma_{284}\gamma_{189}}$$

$$\alpha_{317} = \frac{\gamma_{285}}{\gamma_{284}\gamma_{17}}$$

$$\alpha_{324} = \frac{\gamma_{292}}{\gamma_{284}\gamma_{189}}$$

$$\alpha_{318} = \frac{\gamma_{286}}{\gamma_{284}\gamma_{17}^2}$$

$$\alpha_{325} = \frac{\gamma_{293}}{\gamma_{284}\gamma_{189}}$$

Appendix 3. (cont'd).

$$\alpha_{326} = \frac{\gamma_{294}}{\gamma_{284}\gamma_{236}}$$

$$\alpha_{334} = \frac{\gamma_{302}}{\gamma_{284}\gamma_{62}}$$

$$\alpha_{327} = \frac{\gamma_{295}}{\gamma_{284}\gamma_{236}}$$

$$\alpha_{335} = \frac{\gamma_{303}}{\gamma_{284}\gamma_{62}^2}$$

$$\alpha_{328} = \frac{\gamma_{296}}{\gamma_{284}\gamma_{236}}$$

$$\alpha_{336} = \frac{\gamma_{304}}{\gamma_{284}\gamma_{62}^3}$$

$$\alpha_{329} = \frac{\gamma_{297}}{\gamma_{284}\gamma_{236}}$$

$$\alpha_{337} = 1$$

$$\alpha_{330} = \frac{\gamma_{298}}{\gamma_{284}\gamma_{38}}$$

$$\alpha_{338} = \frac{\gamma_{285}}{\gamma_{284}\gamma_{17}}$$

$$\alpha_{331} = \frac{\gamma_{299}}{\gamma_{284}\gamma_1}$$

$$\alpha_{339} = \frac{\gamma_{285}}{\gamma_{284}\gamma_{17}}$$

$$\alpha_{332} = \frac{\gamma_{300}}{\gamma_{284}\gamma_6}$$

$$\alpha_{340} = \frac{\gamma_{285}}{\gamma_{284}\gamma_{17}}$$

$$\alpha_{333} = \frac{\gamma_{301}}{\gamma_{284}\gamma_6^2}$$

Appendix 3. (cont'd).

$$\alpha_{341} = \frac{\gamma_{285}}{\gamma_{284}\gamma_{17}}$$

$$\alpha_{349} = \frac{\gamma_{314}}{\gamma_{18}\gamma_{306}}$$

$$\alpha_{342} = \frac{1}{\gamma_{306}}$$

$$\alpha_{350} = \frac{\gamma_{315}}{\gamma_{103}\gamma_{306}}$$

$$\alpha_{343} = \frac{\gamma_{308}}{\gamma_{284}\gamma_{306}}$$

$$\alpha_{351} = \frac{\gamma_{316}}{\gamma_{180}\gamma_{306}}$$

$$\alpha_{344} = \frac{\gamma_{309}}{\gamma_{284}\gamma_{306}^2}$$

$$\alpha_{352} = \frac{\gamma_{317}}{\gamma_{184}\gamma_{306}}$$

$$\alpha_{345} = \frac{\gamma_{310}}{\gamma_{284}\gamma_{306}^3}$$

$$\alpha_{353} = \frac{\gamma_{318}}{\gamma_{184}\gamma_{306}^2}$$

$$\alpha_{346} = \frac{\gamma_{311}}{\gamma_{284}\gamma_{306}^4}$$

$$\alpha_{354} = \gamma \frac{319}{\gamma_{184}\gamma_{306}^3}$$

$$\alpha_{347} = \frac{\gamma_{312}}{\gamma_5\gamma_{306}}$$

$$\alpha_{355} = \gamma_5\gamma_{306}^2$$

$$\alpha_{348} = \frac{\gamma_{313}}{\gamma_3\gamma_{306}}$$

$$\alpha_{356} = \gamma_3\gamma_{306}^2$$

Appendix 4. Coefficients (C, m)

K	C	m	References
K ₁	-8.971	-1679.85	9, p. 148 K(t)
K ₂	-16.402	-2198.43	9, p. 148 K(t)
K ₃	-5.3	0	2, p. 136
K ₄	-7.25	0	5, p. 37
K ₅	-6.63	0	5, p. 37
K ₆	-28.7422	2802.8	9, p. 170
K ₇	-38.45	0	9, p. 75
K ₈	-8.825	1944.475	11 M ₁
K ₉	-7.5838	1628.4108	11 M ₂
K ₁₀	-5.18	0	2, p. 136
K ₁₁	-12.063	2589.56	8 K(t)
K ₁₂	0	0	
K ₁₃	-2.99	0	1, p. 42
K ₁₄	-5.94	0	1, p. 42
K ₁₅	12.20083	-2270.69147	12, p. 201 K(t)
K ₁₆	-6.91	0	
K ₁₇	-8.92436	-6948.7892	12, p. 214
K ₁₈	15.50	0	2, p. 77
K ₁₉	23.05	0	1, p. 140
K ₂₀	-46.86	0	2, p. 26
K ₂₁	-17.72	0	5, p. 9
K ₂₂	-31.50	0	1, p. 59
K ₂₃	-61.71	0	3, p. 220
K ₂₄	-91.18	0	5, p. 6
K ₂₅	-24.34	0	2, p. 26
K ₂₆	5.41	0	2, p. 142
K ₂₇	28.32	0	
K ₂₈	0.92	0	1, p. 286
K ₂₉	0.26	0	1, p. 286
K ₃₀	-44.49	0	2, p. 26
K ₃₁	9.31	0	5, p. 41

K	C	m	References
K_{32}	17.20	0	5, p.41
K_{33}	23.60	0	5, p.41
K_{34}	0	0	
K_{35}	-0.1272	-6307.3040	10 K(t)
K_{36}	5.14	0	2, p. 251
K_{37}	8.36	0	2, p. 251
K_{38}	10.95	0	6, p. 3
K_{39}	-22.18	0	1, p. 140
K_{40}	-33.042	0	1, p. 26
K_{41}	-23.26	0	5, p. 9
K_{42}	-46.74	0	5, p. 9
K_{43}	-77.41	0	5, p. 9
K_{44}	-109.6	0	
K_{45}	-21.64	0	5, p. 9
K_{46}	5.66	0	5, p. 84
K_{47}	4.56	0	5, p. 108
K_{48}	5.99	0	5, p. 108
K_{49}	5.53	0	5, p. 108
K_{50}	5.87	0	5, p. 41
K_{51}	10.49	0	5, p. 41
K_{52}	13.58	0	5, p. 41
K_{53}	7.39528	-730.25329	12, p. 189 K(t)
K_{54}	14.056079	751.986802	12, p. 190 K(t)
K_{55}	28.43	0	5, p. 56
K_{56}	4.44	0	6, p. 6
K_{57}	7.25	0	6, p. 6
K_{58}	4.99	0	6, p. 6
K_{59}	6.460156	2906.59766	1, p. 216 K(t)
K_{60}	19.655518	3682.25497	1, p. 217 M ₄
K_{61}	-62.17	0	5, p. 77
K_{62}	-31.64	0	1, p. 146
K_{63}	-83.12	0	5, p. 76

K	C	m	References
K ₆₄	-111.7	0	5, p. 76
K ₆₅	-77.78	0	1, p. 140
K ₆₆	-105.827	0	1, p. 140
K ₆₇	-84.96	0	1, p. 186
K ₆₈	-75.07	0	1, p. 186
K ₆₉	-157.68	0	7, II-4-H-2
K ₇₀	-79.53	0	7, II-4-H-2
K ₇₁	0	0	
K ₇₂	14.873	0	5, p. 56
K ₇₃	6.310	0	5, p. 56
K ₇₄	3.463	0	13, p. 477
K ₇₅	-134.305	0	13, p. 476
K ₇₆	-15.151	0	5, p. 56
K ₇₇	-66.593	0	13, p. 476
K ₇₈	-107.998	0	13, p. 476
K ₇₉	13.82	0	5, p. 56
K ₈₀	6.701	0	5, p. 56
K ₈₁	1.84	0	5, p. 56
K ₈₂	-119.73	0	5, p. 56
K ₈₃	-13.403	0	5, p. 56
K ₈₄	-58.025	0	5, p. 56
K ₈₅	-96.25	0	5, p. 56
K ₈₆	0.5347	-6679.975	
K ₈₇	0.9560	-14420.333	
K ₈₈	-17.9253	-16617.333	
K ₈₉	22.105	0	5, p. 5
K ₉₀	5.066	0	5, p. 82
K ₉₁	8.289	0	5, p. 56
K ₉₂	8.289	0	5, p. 56
K ₉₃	3.224	0	5, p. 5
K ₉₄	-22.6900	-5283.6	14 and ΔH_r
K ₉₅	-26.7355	-2395.166	5, p. 5

K	C	m	References
K ₉₆	-82.783	0	5, p. 57
K ₉₇	-34.9542	3089.648	5, p. 37
K ₉₈	17.458	0	5, p. 77
K ₉₉	34.26	0	5, p. 77
K ₁₀₀	38.64	0	5, p. 77
K ₁₀₁	24.407	0	5, p. 9
K ₁₀₂	50.196	0	5, p. 9
K ₁₀₃	48.124	0	5, p. 9
K ₁₀₄	24.637	0	5, p. 9
K ₁₀₅	81.972	0	5, p. 9
K ₁₀₆	-20.380	0	5, eqn. subst.
K ₁₀₇	8.566	0	electroneg.
K ₁₀₈	29.795	0	5, eqn. subst.
K ₁₀₉	32.236	0	electroneg.
K ₁₁₀	19.895	0	5 (23°C)
K ₁₁₁	39.239	0	5, graphic extrapol.
K ₁₁₂	41.171	0	5, graphic extrapol.
K ₁₁₃	12.134 (30°C)	0	5, graphic extrapol.
K ₁₁₄	21.851 (30°C)	0	5, graphic extrapol.
K ₁₁₅	31.154 (30 °C)	0	5, graphic extrapol.
K ₁₁₆	86.891 (20 °C)	0	5, p. 77
K ₁₁₇	3.086 (I = 0.5)	0	5, p. 84
K ₁₁₈	5.525 (I = 0.5)	0	5, p. 84
K ₁₁₉	0	0	
K ₁₂₀	-23.162	-10559.4	5, p. 9 and ΔH_r
K ₁₂₁	-17.386	-30996.5	5, p. 87 and ΔH_r
K ₁₂₂	-16.909	-31549.8	5, p. 87 and ΔH_r
K ₁₂₃	16.3295	644.08	5, p. 91 and ΔH_r
K ₁₂₄	8.3784	-850.3911	5, p. 91 and ΔH_r
K ₁₂₅	5.0626	0	5, p. 91 (graphic extrapol.)
K ₁₂₆	18.7428	0	5, p. 91 "

K	C	m	References
K ₁₂₇	29.7266	0	5, p. 91 "
K ₁₂₈	11.8277	0	5, p. 91 "
K ₁₂₉	-31.9069	0	5, p. 91 (corr. I = 0)
K ₁₃₀	-17.9149 (20°C)	0	5, p. 91
K ₁₃₁	-12.3418 (20°C)	0	5, p. 91
K ₁₃₂	7.8794	-15.10	5, p. 5
K ₁₃₃	17.7299	0	5, p. 5
K ₁₃₄	7.8288	0	5, p. 5
K ₁₃₅	41.6768	0	5, p. 5
K ₁₃₆	4.1447	0	5, p. 37
K ₁₃₇	10.9093	-1700.14	5, p. 82
K ₁₃₈	0.0967	0	5, p. 105
K ₁₃₉	3.2236	0	6, p. 5
K ₁₄₀	2.3026	0	5, p. 40
K ₁₄₁	3.5460	0	5, p. 40
K ₁₄₂	3.9144	0	5, p. 40
K ₁₄₃	11.5129	0	5, p. 9
K ₁₄₄	25.5586	0	5, p. 9
K ₁₄₅	31.3152	0	5, p. 9
K ₁₄₆	11.5129	0	5, p. 9
K ₁₄₇	5.526	0	5, p. 57
K ₁₄₈	6.5163	0	5, p. 57
K ₁₄₉	5.4801	0	5, p. 84
K ₁₅₀	5.9867	0	5, p. 84
K ₁₅₁	3.4539	0	5, p. 84
K ₁₅₂	0.9901	0	5, p. 108
K ₁₅₃	2.87823	0	5, p. 108
K ₁₅₄	1.1513	0	5, p. 108
K ₁₅₅	3.6151	0	6, p. 6
K ₁₅₆	2.9289	60.36	6, p. 6
K ₁₅₇	4.4210	0	6, p. 6
K ₁₅₈	5.0887	0	5, p. 41

K	C	m	References
K ₁₅₉	10.3616	0	5, p. 41
K ₁₆₀	15.7957	0	5, p. 41
K ₁₆₁	10.5204	11013.185	5, p. 76
K ₁₆₂	-0.4605	0	5, p. 1
K ₁₆₃	3.2236	0	5, p. 56
K ₁₆₄	1.6118	0	5, p. 79
K ₁₆₅	-0.4145	0	6, p. 3
K ₁₆₆	-1.1513	0	5, p. 1
K ₁₆₇	2.7516	0	5, p. 56
K ₁₆₈	1.9572	0	5, p. 79
K ₁₆₉	-1.6118	0	5, p. 104
K ₁₇₀	40.0650	0	5, p. 8
K ₁₇₁	11.9734	0	5, p. 83
K ₁₇₂	16.3023	0	5, p. 83
K ₁₇₃	22.2476	1473.7900	5, p. 7
K ₁₇₄	51.3476	0	5, p. 7
K ₁₇₅	57.795	0	5, p. 7
K ₁₇₆	114.4385	0	5, p. 7
K ₁₇₇	19.11	0	5, p. 57
K ₁₇₈	7.98997	0	5, p. 57
K ₁₇₉	19.8018	-3128.6600	5, p. 79
K ₁₈₀	12.3879	0	5, p. 83
K ₁₈₁	17.6292	-4237.7750	5, p. 106
K ₁₈₂	4.9045	0	5, p. 106
K ₁₈₃	-1.8703	22.1320	5, p. 106
K ₁₈₄	7.8518	0	6, p. 5
K ₁₈₅	15.0129	0	6, p. 5
K ₁₈₆	19.572	0	6, p. 5
K ₁₈₇	6.8732	0	5, p. 91
K ₁₈₈	20.49	0	5, p. 39
K ₁₈₉	22.7773	0	5, p. 39
K ₁₉₀	30.1639	0	5, p. 39

K	C	m	References
K ₁₉₁	60.2356	0	5, p. 39
K ₁₉₂	128.7145	0	5, p. 39
K ₁₉₃	160.000	0	5, p. 39
K ₁₉₄	11.3057	0	5, p. 39
K ₁₉₅	1.6648	0	5, p. 39
K ₁₉₆	8.5426	0	5, p. 39
K ₁₉₇	8.3814	0	5, p. 39
K ₁₉₈	1.0131	0	5, p. 39
K ₁₉₉	6.6545	0	5, p. 39
K ₂₀₀	-89.3403	0	5, p. 39
K ₂₀₁	-23.5661	-1761.2000	5, p. 1
K ₂₀₂	-27.3209	1761.2000	5, p. 37
K ₂₀₃	-13.6458	-3140.0	5, p. 79
K ₂₀₄	-20.3448	-3190.3	5, p. 76
K ₂₀₅	-16.7398	0	5, p. 91
K ₂₀₆	-24.2934	-3411.700	5, p. 9
K ₂₀₇	-30.2010	-2432.97	5, p. 79
K ₂₀₈	-23.0259	0	5, p. 38
K ₂₀₉	-131.304	14914.4	5, p. 57
K ₂₁₀	-18.6448	-9887.9	5, p. 76
K ₂₁₁	-16.5786	0	5, p. 39
K ₂₁₂	-41.2393	0	5, p. 107
K ₂₁₃	-89.3403	0	5, p. 7
K ₂₁₄	-95.5573	0	5, p. 7
K ₂₁₅	-98.3204	0	5, p. 7
K ₂₁₆	-36.9565	0	5, p. 38
K ₂₁₇	-60.7882	0	5, p. 57
K ₂₁₈	-28.5521	0	5, p. 57
K ₂₁₉	-14.1148	0	5, p. 57
K ₂₂₀	0	0	
K ₂₂₁	15.6285	2853.0719	15, p. 204
K ₂₂₂	7.1031	2183.8328	15, p. 204

K	C	m	References
K ₂₂₃	9.2647	-704.4622	15, p. 204
K ₂₂₄	5.8569	-150.9562	15, p. 204
K ₂₂₅	2.1561	704.4622	15, p. 204
K ₂₂₆	27.0070	-1761.1555	15, p. 204
K ₂₂₇	8.1281	0	15, p. 204
K ₂₂₈	14.0000	3321.0360	15, p. 204
K ₂₂₉	6.5844	0	15, p. 204
K ₂₃₀	37.9346	6038.2474	15, p. 207
K ₂₃₁	3.7302	0	15, p. 207
K ₂₃₂	0.8189	5031.8728	15, p. 207
K ₂₃₃	22.4042	0	15, p. 207
K ₂₃₄	19.6764	2515.9364	15, p. 207
K ₂₃₅	18.2625	9510.2396	15, p. 208
K ₂₃₆	6.6733	352.2311	15, p. 208
K ₂₃₇	21.7134	0	15, p. 208
K ₂₃₈	23.0179	4579.0043	15, p. 208
K ₂₃₉	6.7278	201.2749	15, p. 208
K ₂₄₀	29.9507	4126.1357	15, p. 207
K ₂₄₁	4.2117	1006.3746	15, p. 207
K ₂₄₂	1.3440	1509.5618	15, p. 207
K ₂₄₃	26.8441	2012.7491	15, p. 206
K ₂₄₄	3.6361	1006.3746	15, p. 206
K ₂₄₅	21.6213	0	15, p. 206
K ₂₄₆	23.3943	0	15, p. 206
K ₂₄₇	24.7781	2314.6615	15, p. 206
K ₂₄₈	5.82	603.8247	15, p. 206
K ₂₄₉	30.3190	2465.6177	15, p. 208
K ₂₅₀	3.8684	1107.0120	15, p. 208
K ₂₅₁	7.6503	0	15, p. 208
K ₂₅₂	2.5789	0	15, p. 204
K ₂₅₃	31.0830	2113.3866	15, p. 206
K ₂₅₄	4.3834	956.0558	15, p. 206

K	C	m	References
K ₂₅₅	9.9011	0	5, p. 6
K ₂₅₆	19.3417	0	5, p. 6
K ₂₅₇	22.3351	0	5, p. 6
K ₂₅₈	23.4864	0	5, p. 6
K ₂₅₉	6.2170	0	5, p. 6
K ₂₆₀	7.7968	-704.4622	5, p. 82
K ₂₆₁	-0.8183	1610.1993	5, p. 40
K ₂₆₂	8.0590	0	5, p. 40
K ₂₆₃	10.2005	0	5, p. 40
K ₂₆₄ * I=0.1	5.0196	0	5, p. 57
K ₂₆₅	3.3618	0	16, p. 5
K ₂₆₆	15.8994	2314.6615	15, p. 139
K ₂₆₇	7.1129	-100.6375	15, p. 139
K ₂₆₈	4.4879	-100.6375	15, p. 139
K ₂₆₉	22.6342	-2214.0240	15, p. 139
K ₂₇₀	15.1151	704.4622	15, p. 139
K ₂₇₁	9.6377	3924.8608	15, p. 139
K ₂₇₂	21.8055	0	15, p. 141
K ₂₇₃	33.1802	0	15, p. 141
K ₂₇₄	8.0821	0	15, p. 141
K ₂₇₅	27.0323	0	15, p. 141
K ₂₇₆	26.3541	50.3187	15, p. 141
K ₂₇₇	27.5203	2415.2990	15, p. 141
K ₂₇₈	8.2898	5535.0601	15, p. 141
K ₂₇₉	29.2052	956.0558	15, p. 141
K ₂₈₀	27.4828	4478.3668	15, p. 141
K ₂₈₁	12.4240	0	15, p. 142
K ₂₈₂	0	0	
K ₂₈₃	44.7286	-1610.1993	15, p. 142
K ₂₈₄	58.5778	0	15, p. 142
K ₂₈₅	12.0655	0	15, p. 142
K ₂₈₆	20.5851	0	15, p. 142

K	C	m	References
K ₂₈₇	25.6487	452.8686	15, p. 142
K ₂₈₈	29.3498	1811.4742	15, p. 142
K ₂₈₉	10.4998	0	15, p. 142
K ₂₉₀	0	0	
K ₂₉₁	18.3937	2012.7491	15, p. 142
K ₂₉₂	20.6462	4579.0043	15, p. 142
K ₂₉₃	9.3260	5535.0601	15, p. 142
K ₂₉₄	36.2427	0	15, p. 143
K ₂₉₅	5.4341	0	15, p. 139
K ₂₉₆	22.1592	-704.4622	15, p. 141
K ₂₉₇	20.8930	2063.0679	15, p. 141
K ₂₉₈	-22.9798	0	5, p. 38
K ₂₉₉	-34.3085	0	5, p. 6
K ₃₀₀	-79.8997	0	1, p. 186
K ₃₀₁	-49.0451	0	4, p. 76
K ₃₀₂	22.7035	0	
K ₃₀₃	30.1639	0	
K ₃₀₄	0	0	
K ₃₀₅	0	0	
K ₃₀₆	0	0	
K ₃₀₇	0	0	
K ₃₀₈	0	0	
K ₃₀₉	0	0	
K ₃₁₀	0	0	
K ₃₁₁	0	0	
K ₃₁₂	0	0	
K ₃₁₃	0	0	
K ₃₁₄	0	0	
K ₃₁₅	0	0	
K ₃₁₆	0	0	
K ₃₁₇	20.7431	0	
K ₃₁₈	43.058	0	

K	C	m	References
K ₃₁₉	62.1698	0	
K ₃₂₀	75.9853	0	
K ₃₂₁	46.7448	0	
K ₃₂₂	96.9397	0	
K ₃₂₃	37.5345	0	
K ₃₂₄	43.2897	0	
K ₃₂₅	23.9698	0	
K ₃₂₆	26.2487	0	
K ₃₂₇	30.6268	0	
K ₃₂₈	13.4702	0	
K ₃₂₉	-6.8124	0	
K ₃₃₀	3.4769	0	
K ₃₃₁	19.4102	0	
K ₃₃₂	7.3652	0	
K ₃₃₃	11.7440	0	
K ₃₃₄	6.9078	0	
K ₃₃₅	12.2061	0	
K ₃₃₆	17.4994	0	
K ₃₃₇	0	0	
K ₃₃₈	-77.1371	0	
K ₃₃₉	-71.8171	0	
K ₃₄₀	-41.9999	0	
K ₃₄₁	-68.0408	0	
K ₃₄₂	7.2991	0	
K ₃₄₃	16.1181	0	
K ₃₄₄	29.0123	0	
K ₃₄₅	38.4528	0	
K ₃₄₆	43.9794	0	
K ₃₄₇	4.1447	0	
K ₃₄₈	2.5329	0	
K ₃₄₉	2.7632	0	
K ₃₅₀	3.6841	0	

K	C	m	References
K_{351}	2.6479	0	
K_{352}	13.8155	0	
K_{353}	24.1764	0	
K_{354}	29.9336	0	
K_{355}	-18.8351	0	
K_{356}	-23.9699	0	

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