# Thermodynamics of Enzyme-Catalyzed Reactions: Part 6—1999 Update

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This review serves to update previously published evaluations of equilibrium constants and enthalpy changes for enzyme-catalyzed reactions. For each reaction the following information is given: the reference for the data; the reaction studied; the name of the enzyme used and its Enzyme Commission number; the method of measurement; the conditions of measurement [temperature, pH, ionic strength, and the buffer(s) and cofactor(s) used]; the data and an evaluation of it; and, sometimes, commentary on the data and on any corrections which have been applied to it or any calculations for which the data have been used. The data from 96 references have been examined and evaluated. Chemical Abstract Service registry numbers are given for the substances involved in these various reactions. There is also a cross reference between the substances and the Enzyme Commission numbers of the enzymes used to catalyze the reactions in which the substances participate. © *1999 American Institute of Physics and American Chemical Society.* [S0047-2689(99)00204-4]

Key words: apparent equilibrium constants; enthalpies of reaction; enzyme-catalyzed reactions; evaluated data; transformed thermodynamic properties.

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## 1. Introduction

This paper serves to update a series of reviews[1–5] on the thermodynamics of enzyme-catalyzed reactions. These reviews, which were published during the years 1993–1995, deal with the thermodynamics of the reactions catalyzed by the six classes of enzymes classified by the Nomenclature Committee of the International Union of Biochemistry:[6] oxidoreductases,[1] transferases,[2] hydrolases,[3] lyases,[4] isomerases,[5] and ligases.[5] The current review updates these earlier publications by providing coverage of the literature through the end of 1998. Thus, while it primarily consists of papers published since the completion of the earlier reviews,[1–5] additional papers which contain data missed previously are also included. Accordingly, it is important that anyone examining a given reaction for which data are given in this review, also consult the earlier reviews[1–5] in order to determine if more reliable results have been previously summarized.

Enzyme-catalyzed reactions play significant roles in many biological processes such as glycolysis, the anabolism and catabolism of carbohydrates, fermentation, and vision. Many of these reactions are also of current or potential importance for the production of pharmaceuticals and bulk commodity chemicals such as ethanol, fructose, and amino acids. The data presented herein are limited to equilibrium and calorimetric measurements performed on these reactions under *in vitro* conditions. Thus, the thermodynamic quantities which are generally given are apparent equilibrium constants $K'$ and calorimetrically determined enthalpies of reaction $\Delta_r H(\text{cal})$. Apparent equilibrium constants calculated from kinetic data are also tabulated. If the change in binding of hydrogen ion $\Delta_r N(H^+)$ in a biochemical reaction and the enthalpy of protonation of the buffer are known, the standard transformed enthalpy of reaction $\Delta_r H'^\circ$ can be calculated from the calorimetrically determined enthalpy of reaction.[7] Equilibrium constants $K$ and standard molar enthalpies of reaction $\Delta_r H^\circ$ for chemical reference reactions are also

given if they have been reported in the literature. The standard transformed enthalpy of reaction $\Delta_r H'^\circ$ can be used to calculate the temperature dependence of apparent equilibrium constants $K'$ in the same way that the standard enthalpy of reaction $\Delta_r H^\circ$ is used to calculate the temperature dependence of the equilibrium constant $K$.

These data also serve as a basis for many additional thermodynamic calculations. Thus, Alberty[8,9] has used data given in the previous reviews[1–5] to calculate tables of standard transformed formation properties that are useful for the calculation of apparent equilibrium constants $K'$ and standard transformed enthalpies of reaction $\Delta_r H'^\circ$ under specified conditions of temperature, pH, pMg, and ionic strength. If the prerequisite thermodynamic quantities on the binding of $H^+$(aq) and metal ions are available, it is also possible to calculate standard thermodynamic quantities ($K$ and $\Delta_r H^\circ$) for reference reactions that involve specific species. Such calculations serve to transform the results of measurements made under varied conditions and that pertain to a mixture of species to results for reference reactions that pertain to the same standard state. Thus, once a sufficiently large reaction catalog has been established, thermodynamic network calculations[10] can be performed both to check the consistency of the data and to calculate "best" values of standard formation properties. Finally, and most importantly, these standard formation properties can then be used to calculate values of $K$ and $\Delta_r H^\circ$ for a very large number of reactions that have not been the subject of investigation.

The data are presented in the same format as in the previous reviews.[1–5] Thus, the following information is given for each entry in this review: the reference for the data; the biochemical reaction studied; the name of the enzyme used and its Enzyme Commission number; the method of measurement; the conditions of measurement [temperature, pH, ionic strength, and the buffer(s) and cofactor(s) used]; the data and an evaluation of it; and, sometimes, commentary on the data and on any corrections which have been applied to it or any calculations for which the data have been used. The absence of a piece of information indicates that it was not found in the paper cited. The arrangement of the data, its evaluation, and the thermodynamic conventions have been discussed previously.[1] In this regard, one should express equilibrium constants as dimensionless quantities. However, the numerical value obtained for the equilibrium constant of an unsymmetrical reaction will depend upon the measure of composition and standard concentration selected for the reactants and products. Thus, for the chemical reaction

$$\mathrm{A(aq)=B(aq)+C(aq)}, \qquad (1)$$

$K_c=c(\mathrm{B})c(\mathrm{C})/\{c(\mathrm{A})c^\circ\}$, $K_m=m(\mathrm{B})m(\mathrm{C})/\{m(\mathrm{A})m^\circ\}$, and $K_x=x(\mathrm{B})x(\mathrm{C})/x(\mathrm{A})$. Here, $c$, $m$, and $x$ are, respectively, concentration, molality, and mole fraction, $c^\circ=1\ \mathrm{mol\,dm^{-3}}$, and $m^\circ=1\ \mathrm{mol\,kg^{-1}}$. The equilibrium constant expressed in terms of mole fractions is automatically dimensionless. Similar definitions and considerations apply to the apparent equilibrium constant $K'$. The symbols used in this paper are given in the Glossary (see Sec. 7).

The *subjective* evaluation of the data in this review consisted of the assignment of a rating: A (high quality), B(good), C (average), or D (low quality). In making these assignments, we considered the various experimental details which were provided in the study. These details include the method of measurement, the number of data points determined, and the extent to which the effects of varying temperature, pH, and ionic strength were investigated. A lower rating was generally given when few details of the investigation were reported. For example, in many of the papers cited, the major aim of the study was the isolation and purification of the enzyme of interest. Thus, the equilibrium data were obtained as only a small part of an investigation to characterize many of the properties of that enzyme and the reaction it catalyzes.

This effort began $\approx$10 years ago with an extensive search of the literature to locate the papers containing the relevant data. This search was based on a carefully designed computer search of Chemical Abstracts, a manual search of Methods in Enzymology, and the examination of references found in earlier reviews that dealt with the thermodynamics of enzyme-catalyzed reactions.[11–21] The references obtained from these sources were in turn examined for additional references relevant to this effort. The current update, which covers the literature through the end of 1998, relied primarily on a search of Chemical Abstracts. The author would be most grateful if references that contain data on the thermodynamics of enzyme-catalyzed reactions that were not included in these reviews were brought to his attention.

## 2. Acknowledgments

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## 3. References for the Introductory Discussion

[1] R. N. Goldberg, Y. B. Tewari, D. Bell, K. Fazio, and E. Anderson, J. Phys. Chem. Ref. Data **22**, 515 (1993).
[2] R. N. Goldberg and Y. B. Tewari, J. Phys. Chem. Ref. Data **23**, 547 (1994).
[3] R. N. Goldberg and Y. B. Tewari, J. Phys. Chem. Ref. Data **23**, 1035 (1994).
[4] R. N. Goldberg and Y. B. Tewari, J. Phys. Chem. Ref. Data **24**, 1669 (1995).
[5] R. N. Goldberg and Y. B. Tewari, J. Phys. Chem. Ref. Data **24**, 1765 (1995).
[6] E. C. Webb, *Enzyme Nomenclature 1992* (Academic, San Diego, 1992).
[7] R. A. Alberty and R. N. Goldberg, Biophys. Chem. **47**, 213 (1993).
[8] R. A. Alberty, Arch. Biochem. Biophys. **353**, 116 (1998).
[9] R. A. Alberty, Arch. Biochem. Biophys. **358**, 25 (1998).
[10] R. N. Goldberg and Y. B. Tewari, J. Phys. Chem. Ref. Data **18**, 809 (1989).
[11] H. A. Krebs and H. L. Kornberg, with an appendix by K. Burton, *A Survey of the Energy Transformations in Living Matter* (Springer, Berlin, 1957).
[12] M. R. Atkinson and R. K. Morton, in *Comparative Biochemistry*, edited

by M. Florkin and H. S. Mason (Academic, New York, 1960), Vol. 2, pp. 1–95.
[13] J. M. Sturtevant, in *Experimental Thermochemistry*, Volume II, edited by H. A. Skinner (Interscience, New York, 1962).
[14] T. E. Barman, *Enzyme Handbook* (Springer, New York, 1969), Vols. I and II.
[15] T. E. Barman, *Enzyme Handbook* (Springer, New York, 1974), Supplement I.
[16] H. D. Brown, in *Biochemical Microcalorimetry*, edited by H. D. Brown (Academic, New York, 1969), pp. 149–164.
[17] R. C. Wilhoit, in *Biochemical Microcalorimetry*, edited by H. D. Brown (Academic, New York, 1969), pp. 33–81, 305–317.
[18] R. K. Thauer, K. Jungermann, and K. Decker, Bacteriol. Rev. **41**, 100 (1977).
[19] M. V. Rekharsky, A. M. Egorov, G. L. Gal'chenko, and I. V. Berezin, Thermochim. Acta **46**, 89 (1981).
[20] M. V. Rekharsky, G. L. Gal'chenko, A. M. Egorov, and I. V. Berezin, in *Thermodynamic Data for Biochemistry and Biotechnology*, edited by H. J. Hinz (Springer, Berlin, 1986), pp. 431–444.
[21] S. L. Miller and D. Smith-Magowan, J. Phys. Chem. Ref. Data **19**, 1049 (1990).

## 4. Table of Equilibrium Constants and Enthalpies of Reaction

### 4.1. Enzyme: alcohol dehydrogenase (EC 1.1.1.1)

ethanol(aq)+NAD(aq)=acetaldehyde(aq)+NADH(aq)

| $T$/K | $P$/MPa | pH | $K'$ |
|---|---|---|---|
| 298.15 | 0.1 | 8.8 | 4.23 |
| 298.15 | 30 | 8.8 | 2.54 |
| 298.15 | 60 | 8.8 | 1.84 |
| 298.15 | 90 | 8.8 | 1.73 |
| 298.15 | 120 | 8.8 | 1.33 |
| 298.15 | 150 | 8.8 | 1.27 |
| 308.15 | 0.1 | 8.8 | 1.81 |
| 308.15 | 30 | 8.8 | 1.98 |
| 308.15 | 60 | 8.8 | 1.73 |
| 308.15 | 90 | 8.8 | 1.60 |
| 308.15 | 120 | 8.8 | 1.08 |
| 308.15 | 150 | 8.8 | 1.22 |

Reference: 89JEE/SHI
Method: spectrophotometry
Buffer: Tris ($0.1\,\mathrm{mol\,dm^{-3}}$)+HCl
pH: 8.8
Evaluation: D

Jee and Shin measured the apparent equilibrium constant $K'$ as a function of pressure $P$. The reported pH is that of the buffer at $P=0.1$ MPa. This may have caused a systematic error in the results since the apparent equilibrium constant is a function of pH. Also, the reported values differ significantly from several previously reported results (see for example the results of Backlin [58BAC] and Burton [74BUR] summarized by Goldberg *et al.* [93GOL/TEW]) which were judged to be reliable. Thus, the results of Jee and Shin [89JEE/SHI] are considered to be in error.

### 4.2. Enzyme: L-iditol 2-dehydrogenase (EC 1.1.1.14)

D-arabitol(aq)+NAD(aq)=D-ribulose(aq)+NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 0.0008 |

Reference: 89SCH/GIF
Method: spectrophotometry
Buffer: potassium phosphate ($0.10\,\mathrm{mol\,dm^{-3}}$)
pH: 7.0
Evaluation: C

Schneider and Giffhorn reported $K'c(\mathrm{H^+})/c^\circ = 8.0\cdot 10^{-11}$ at pH=7.0. The apparent equilibrium constant given here was calculated from this result.

L-iditol(aq)+NAD(aq)=L-sorbose(aq)+NADH(aq)

| $T$/K | pH | $I_m$ / mol·kg$^{-1}$ | $K'$ |
|---|---|---|---|
| 298.15 | 7.58 | 0.191 | 0.186 |

Reference: 96TEW/GOL
Method: HPLC and spectrophotometry
Buffer: phosphate
pH: 7.58
Evaluation: A

Tewari and Goldberg also calculated $K=2.02\cdot 10^{-9}$ and $\Delta_r H^\circ = 14.7\,\mathrm{kJ\,mol^{-1}}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-iditol(aq)+$\mathrm{NAD^-}$(aq)=L-sorbose(aq)+$\mathrm{NADH^{2-}}$(aq)+$\mathrm{H^+}$(aq).

L-iditol(aq)+NAD(aq)=L-sorbose(aq)+NADH(aq)

| $T$/K | pH | $I_m$ / mol·kg$^{-1}$ | $\Delta_r H$(cal) / kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 7.39 | 0.215 | −10.5 |

Reference: 96TEW/GOL
Method: calorimetry
Buffer: phosphate
pH: 7.39
Evaluation: A

Tewari and Goldberg also calculated $K=2.02\cdot 10^{-9}$ and $\Delta_r H^\circ = 14.7\,\mathrm{kJ\,mol^{-1}}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-iditol(aq)+$\mathrm{NAD^-}$(aq)=L-sorbose(aq)+$\mathrm{NADH^{2-}}$(aq)+$\mathrm{H^+}$(aq).

D-mannitol(aq)+NAD(aq)=D-fructose(aq)+NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 0.045 |

Reference: 89SCH/GIF
Method: spectrophotometry
Buffer: potassium phosphate (0.10 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Schneider and Giffhorn reported $K'c(H^+)/c^\circ = 4.5 \cdot 10^{-9}$ at pH=7.0. The apparent equilibrium constant given here was calculated from this result.

D-sorbitol(aq)+NAD(aq)=D-fructose(aq)+NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 0.0058 |

Reference: 89SCH/GIF
Method: spectrophotometry
Buffer: potassium phosphate (0.10 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Schneider and Giffhorn reported $K'c(H^+)/c^\circ = 5.8 \cdot 10^{-10}$ at pH=7.0. The apparent equilibrium constant given here was calculated from this result.

D-sorbitol(aq)+NAD(aq)=D-fructose(aq)+NADH(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'$ |
| 298.15 | 7.63 | 0.197 | 0.094 |

Reference: 96TEW/GOL
Method: HPLC and spectrophotometry
Buffer: phosphate
pH: 7.63
Evaluation: A

Tewari and Goldberg also calculated $K = 9.0 \cdot 10^{-10}$ and $\Delta_r H^\circ = 21.3$ kJ mol$^{-1}$ at $T = 298.15$ K and $I = 0$ for the reference reaction: D-sorbitol(aq)+NAD$^-$(aq)=D-fructose(aq) +NADH$^{2-}$(aq)+H$^+$(aq).

D-sorbitol(aq)+NAD(aq)=D-fructose(aq)+NADH(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.55 | 0.217 | −17.1 |

Reference: 96TEW/GOL
Method: calorimetry
Buffer: phosphate
pH: 7.55
Evaluation: A

Tewari and Goldberg also calculated $K = 9.0 \cdot 10^{-10}$ and $\Delta_r H^\circ = 21.3$ kJ mol$^{-1}$ at $T = 298.15$ K and $I = 0$ for the reference reaction: D-sorbitol(aq)+NAD$^-$(aq)=D-fructose(aq) +NADH$^{2-}$(aq)+H$^+$(aq).

xylitol(aq)+NAD(aq)=D-xylulose(aq)+NADH(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'$ |
| 298.15 | 7.51 | 0.189 | 0.00122 |

Reference: 96TEW/GOL
Method: HPLC and spectrophotometry
Buffer: phosphate
pH: 7.51
Evaluation: A

Tewari and Goldberg also calculated $K = 1.53 \cdot 10^{-11}$ and $\Delta_r H^\circ = 39.4$ kJ mol$^{-1}$ at $T = 298.15$ K and $I = 0$ for the reference reaction: xylitol(aq)+NAD$^-$(aq)=D-xylulose(aq) +NADH$^{2-}$($aq$)+H$^+$(aq).

xylitol(aq)+NAD(aq)=D-xylulose(aq)+NADH(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.43 | 0.218 | −35.2 |

Reference: 96TEW/GOL
Method: calorimetry
Buffer: phosphate
pH: 7.43
Evaluation: A

Tewari and Goldberg also calculated $K = 1.53 \cdot 10^{-11}$ and $\Delta_r H^\circ = 39.4$ kJ mol$^{-1}$ at $T = 298.15$ K and $I = 0$ for the reference reaction: xylitol(aq)+NAD$^-$(aq)=D-xylulose(aq) +NADH$^{2-}$(aq)+H$^+$(aq).

### 4.3. Enzyme: L-lactate dehydrogenase (EC 1.1.1.27)

(*S*)-lactate(aq)+NAD(aq)=pyruvate(aq)+NADH(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 7.5 | 41.8 |

Reference: 76SCH/KRI
Method: calorimetry
Buffer: phosphate (0.07 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

### 4.4. Enzyme: ribitol 2-dehydrogenase (EC 1.1.1.56)

ribitol(aq)+NAD(aq)=D-ribulose(aq)+NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 0.0033 |

Reference: 92KAH/SCH
Method: spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Kahle and Schneider report $K'c(H^+)/c^\circ = 3.3 \cdot 10^{-10}$ at pH =7.0. The apparent equilibrium constant given here was calculated from this result.

### 4.5. Enzyme: mannitol 2-dehydrogenase (EC 1.1.1.67)

D-mannitol(aq)+NADP(aq)=D-fructose(aq)+NADPH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 7.5 | 0.0917 |

Reference: 94NOE/COL
Method: HPLC and spectrophotometry
Buffer: Tris (0.020 mol dm$^{-3}$) + HCl
pH: 7.5
Evaluation: B

### 4.6. Enzyme: carnitine 3-dehydrogenase (EC 1.1.1.108)

D-carnitine(aq) + NAD(aq)=3-dehydrocarnitine(aq) +NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 295.15 | 8.0 | 0.00022 |
| 295.15 | 9.0 | 0.0022 |

Reference: 97HAN/KLE
Method: spectrophotometry and HPLC
Buffer: Tris (0.05 mol dm$^{-3}$) + HCl
pH: 8.0–9.0
Evaluation: B

Hanschmann and Kleber report $K'c(H^+)/c^\circ = 2.2 \cdot 10^{-12}$ over the pH range 8.0–9.0. The apparent equilibrium constants given here were calculated from this result.

### 4.7. Enzyme: 15-hydroxyprostaglandin dehydrogenase ($NAD^+$) (EC 1.1.1.141)

prostaglandin $E_2$(aq)+NAD(aq)=15-oxo-prostaglandin $E_2$(aq)+NADH(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | $1.77 \cdot 10^2$ |
| 298.15 | 8.0 | $1.77 \cdot 10^3$ |

Reference: 75SCH/GRE
Method: spectrophotometry
Buffer: Tris (0.1 mol dm$^{-3}$)
pH: 7.0–8.0
Evaluation: C

This approximate result was calculated from kinetic data. Schlegel and Greep reported that $K'c(H^+)/c^\circ = 1.77 \cdot 10^{-5}$ but did not report the pH(s). We have assumed that the pH was in the range 7.0–8.0.

### 4.8. Enzyme: glucose oxidase (EC 1.1.3.4)

β-D-glucose(aq)+$O_2$(aq)=D-glucono-1,5-lactone(aq) +$H_2O_2$(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 6.86 | −125 |

Reference: 93BOH/HUT
Method: calorimetry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 6.86
Evaluation: A

The same result was obtained by Hüttl *et al.* [93HUT/BOH].

β-D-glucose(aq)+$\frac{1}{2}O_2$(aq)=D-glucono-1,5-lactone(aq) +$H_2O$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 300.15 | 7.0 | −207.1 |

Reference: 76SCH/KRI
Method: calorimetry
Buffer: phosphate (0.066 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Catalase (EC 1.11.1.6) was also present.

β-D-glucose(aq)+$\frac{1}{2}O_2$(aq)=D-glucono-1,5-lactone(aq) +$H_2O$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 6.86 | −223 |

Reference: 93HUT/BOH
Method: calorimetry
Buffer: phosphate
pH: 6.86
Evaluation: B

Catalase (EC 1.11.1.6) was also present.

### 4.9. Enzyme: cholesterol oxidase (EC 1.1.3.6)

cholesterol(aq)+$O_2$(aq)=cholest-4-en-3-one(aq)+$H_2O_2$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 303.15 | 7.0 | −114 |

Reference: 78MCG/BRO
Method: calorimetry
Buffer: phosphate (0.067 mol dm$^{-3}$)
pH: 7.0
Evaluation: B

cholesterol(aq)+$\frac{1}{2}O_2$(aq)=cholest-4-en-3-one(aq)+$H_2O$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 303.15 | 7.0 | −214 |

Reference: 78MCG/BRO
Method: calorimetry
Buffer: phosphate (0.067 mol dm$^{-3}$)
pH: 7.0
Evaluation: B

Catalase (EC 1.11.1.6) was also present.

cholesterol(aq)+$\frac{1}{2}O_2$(aq)=cholest-4-en-3-one(aq)+$H_2O$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 303.15 | 6.9 | −153.4 |

Reference: 82REH/YOU
Method: calorimetry
Buffer: phosphate
pH: 6.9
Evaluation: B

Catalase (EC 1.11.1.6) was also present.

### 4.10. Enzyme: prephenate dehydrogenase (EC 1.3.1.12)

prephenate(aq)+NAD(aq)+$H_2O$(l)=4-hydroxyphenylpyruvate(aq)+NADH(aq)+carbon dioxide(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 6.98 | 0.32 | −79.0 |

Reference: 99KIS/HOL
Method: calorimetry
Buffer: phosphate
pH: 6.98
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0)$ = −74 kJ mol$^{-1}$ for the reference reaction: prephenate$^{2-}$(aq)+NAD$^-$(aq)+$H_2O$(l)=4-hydroxyphenylpyruvate$^-$(aq)+NADH$^{2-}$(aq)+$HCO_3^-$(aq)+$H^+$(aq).

### 4.11. Enzyme: dihydrooratate dehydrogenase (1.3.99.11)

(S)-dihydroorotate(aq)+ oxonic acid(aq) = orotate(aq)+ dihydroxonic acid(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 0.040 |

Reference: 98THO/JOR
Method: spectrophotometry
Buffer: sodium phosphate (0.1 mol dm$^{-3}$)
pH: 7.0
Evaluation: B

### 4.12. Enzyme: glycine dehydrogenase (decarboxylating) (EC 1.4.4.2)

glycine(aq)+$\alpha$-lipoate(aq)=(*S*)-aminomethyldihydro-$\alpha$-lipoate(aq)+carbon dioxide(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 311.15 | 6.39 | 0.0310 |
| 311.15 | 6.39 | 0.0222 |
| 311.15 | 6.62 | 0.0221 |
| 311.15 | 6.80 | 0.0301 |
| 311.15 | 6.83 | 0.0465 |
| 311.15 | 6.99 | 0.0511 |
| 311.15 | 6.99 | 0.0328 |
| 311.15 | 6.99 | 0.0344 |
| 311.15 | 7.01 | 0.0302 |
| 311.15 | 7.03 | 0.0140 |
| 311.15 | 7.04 | 0.0121 |
| 311.15 | 7.17 | 0.0240 |
| 311.15 | 7.18 | 0.0197 |
| 311.15 | 7.20 | 0.0229 |
| 311.15 | 7.79 | 0.008 29 |

Reference: 85LIE
Method: spectrophotometry and enzymatic assay
Buffer: phosphate
pH: 6.39–7.79
Evaluation: A

The ionic strength was 0.25 mol dm$^{-3}$.

### 4.13. Enzyme: glutathione reductase (NADPH) (EC 1.6.4.2)

2 reduced glutathione(aq)+NAD(aq)=oxidized glutathione(aq)+NADH(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 313.15 | 7.0 | 0.001 |

Reference: 64ROS/RAP
Method: spectrophotometry
Buffer: phosphate (0.125 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Few details are given in this study.

2 reduced glutathione(aq)+NADP(aq)=oxidized glutathione(aq)+NADPH(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.00 | 0.0053 |
| 298.15 | 7.82 | 0.0373 |
| 298.15 | 8.00 | 0.049 |
| 298.15 | 8.47 | 0.138 |

Reference: 75GOR/ESF
Method: spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$) and Tris (0.1 mol dm$^{-3}$)
pH: 7.0–8.47
Evaluation: A

### 4.14. Enzyme: urate oxidase (EC 1.7.3.3)

urate(aq)+$\frac{1}{2}O_2$(aq)+2 $H_2O$(l)=allantoin(aq)+carbon dioxide(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 303.15 | 9.0 | −149.6 |

Reference: 77REH/JAN
Method: calorimetry
Buffer: Tris (0.02 mol dm$^{-3}$)+HCl
pH: 9.0
Evaluation: B

Catalase (EC 1.11.1.6) was also present.

### 4.15. Enzyme: dihydrolipoamide dehydrogenase (EC 1.8.1.4)

dihydro-$\alpha$-lipoate(aq)+NAD(aq)=$\alpha$-lipoate(aq)+NADH(aq)

| $T$/K | pH | $c(MgCl_2)$ mol·dm$^{-3}$ | $I_c$ mol·dm$^{-3}$ | $K'$ |
|---|---|---|---|---|
| 298.15 | 6.87 | 0 | 0.25 | 0.138 |
| 298.15 | 6.89 | 0 | 0.25 | 0.130 |
| 298.15 | 7.08 | 0 | 0.25 | 0.267 |
| 298.15 | 7.09 | 0 | 0.25 | 0.270 |
| 298.15 | 7.09 | 0 | 0.25 | 0.294 |
| 298.15 | 7.12 | 0 | 0.25 | 0.329 |
| 298.15 | 7.35 | 0 | 0.25 | 0.445 |
| 298.15 | 7.41 | 0 | 0.25 | 0.579 |
| 298.15 | 7.37 | 0 | 0.10 | 0.360 |
| 298.15 | 6.60 | 0 | 0.12 | 0.100 |
| 298.15 | 7.19 | 0 | 0.35 | 0.287 |
| 298.15 | 7.21 | 0 | 0.35 | 0.349 |
| 298.15 | 7.18 | 0 | 0.35 | 0.338 |
| 298.15 | 7.11 | 0 | 0.60 | 0.253 |
| 298.15 | 7.14 | 0 | 0.60 | 0.334 |
| 298.15 | 7.03 | 0 | 1.10 | 0.160 |
| 298.15 | 7.05 | 0 | 1.10 | 0.264 |
| 311.15 | 6.27 | 0 | 0.25 | 0.051 |
| 311.15 | 6.41 | 0 | 0.25 | 0.067 |
| 311.15 | 6.72 | 0 | 0.25 | 0.088 |
| 311.15 | 6.73 | 0 | 0.25 | 0.141 |
| 311.15 | 6.75 | 0 | 0.25 | 0.141 |
| 311.15 | 6.79 | 0 | 0.25 | 0.138 |
| 311.15 | 6.82 | 0 | 0.25 | 0.129 |
| 311.15 | 6.84 | 0 | 0.25 | 0.150 |
| 311.15 | 6.91 | 0 | 0.25 | 0.139 |
| 311.15 | 6.91 | 0 | 0.25 | 0.143 |
| 311.15 | 6.94 | 0 | 0.25 | 0.187 |
| 311.15 | 6.94 | 0 | 0.25 | 0.197 |
| 311.15 | 6.98 | 0 | 0.25 | 0.260 |
| 311.15 | 6.98 | 0 | 0.25 | 0.271 |
| 311.15 | 7.05 | 0 | 0.25 | 0.271 |
| 311.15 | 7.05 | 0.010 | 0.25 | 0.116 |
| 311.15 | 7.06 | 0 | 0.25 | 0.266 |
| 311.15 | 7.07 | 0 | 0.25 | 0.340 |
| 311.15 | 7.07 | 0.010 | 0.25 | 0.105 |
| 311.15 | 7.09 | 0 | 0.25 | 0.328 |
| 311.15 | 7.16 | 0.010 | 0.25 | 0.257 |
| 311.15 | 7.17 | 0 | 0.25 | 0.268 |
| 311.15 | 7.23 | 0 | 0.25 | 0.351 |
| 311.15 | 7.24 | 0 | 0.25 | 0.321 |
| 311.15 | 7.25 | 0 | 0.25 | 0.309 |
| 311.15 | 7.30 | 0 | 0.25 | 0.385 |
| 311.15 | 7.35 | 0 | 0.25 | 0.498 |
| 311.15 | 7.58 | 0 | 0.25 | 0.634 |
| 311.15 | 7.60 | 0 | 0.25 | 0.620 |
| 311.15 | 8.09 | 0 | 0.25 | 2.37 |
| 311.15 | 8.12 | 0 | 0.25 | 2.04 |
| 311.15 | 8.27 | 0 | 0.25 | 3.55 |
| 311.15 | 8.29 | 0 | 0.25 | 2.75 |
| 311.15 | 8.39 | 0 | 0.25 | 3.55 |
| 311.15 | 8.49 | 0 | 0.25 | 3.86 |
| 311.15 | 8.49 | 0 | 0.25 | 6.55 |

Reference: 85LIE
Method: spectrophotometry
Buffer: potassium phosphate (0.050 mol dm$^{-3}$) or sodium pyrophosphate (0.030 mol dm$^{-3}$)
pH: 6.27–8.49
Evaluation: A

Liegel calculated $K(T=311.15\ \text{K},\ I_c\approx 0.25\ \text{mol dm}^{-3}) = 2.08\cdot 10^{-8}$ and $K(T=298.15\ \text{K},\ I_c\approx 0.25\ \text{mol dm}^{-3}) = 2.13\cdot 10^{-8}$ for the reference reaction: dihydro-$\alpha$-lipoate$^-$(aq)+NAD$^-$(aq) = $\alpha$-lipoate$^-$(aq) + NADH$^{2-}$(aq) +H$^+$(aq). Liegel also stated that the earlier measurements of Sanadi *et al.* [59SAN/LAN] may not have been at equilibrium.

### 4.16. Enzyme: catalase (EC 1.11.1.6)

$H_2O_2(aq)=\frac{1}{2}O_2(aq)+H_2O(l)$

| $T$/K | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|
| 298.15 | −100.4 |

Reference: 72NEL/KIE
Method: calorimetry
Buffer: none
pH: not reported
Evaluation: A

Also see entries given under glucose oxidase (EC 1.1.3.4) and cholesterol oxidase (EC 1.1.3.6).

$H_2O_2(aq)=\frac{1}{2}O_2(aq)+H_2O(l)$

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 7.0 | −83.7 |

Reference: 95LIA/WAN
Method: calorimetry
Buffer: phosphate (0.067 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Also see entries given under glucose oxidase (EC 1.1.3.4) and cholesterol oxidase (EC 1.1.3.6).

$H_{22}(aq)=\frac{1}{2}O_2(aq)+H_2O(l)$

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 7.0 | −88.88 |

Reference: 97LIA/WU
Method: calorimetry
Buffer: phosphate
pH: 7.0
Evaluation: B

### 4.17. Enzyme: peroxidase (EC 1.11.1.7)

$H_2O_2(aq)$ +reduced thiocyanate(aq)=oxidized thiocyanate(aq)+$H_2O(l)$

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.0 | $3.8\cdot 10^3$ |

Reference: 86PRU/TEN
Method: enzymatic assay and chemical analysis
Buffer: phosphate
pH: 7.0
Evaluation: B

The value of $K'_c$ given here was calculated from the concentrations given in Pruitt *et al.*'s Table I. Pruitt *et al.* also calculated $K'_c(T=310.15\ \text{K})=3.7\cdot 10^3$ for the reference reaction: $H_2O_2(aq)+SCN^-(aq)=OSCN^-(aq)+H_2O(l)$.

### 4.18. Enzyme: alkanal monooxygenase (FMN-linked) (EC 1.14.14.3)

dodecanal(aq)+reduced riboflavin 5′-phosphate(aq)+$O_2$(aq) =dodecanoic acid(aq)+oxidized riboflavin 5′-phosphate(aq) +$H_2O$(l)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 280.15 | 7.0 | −350 |
| 298.15 | 7.0 | −308 |

Reference: 75MAN/LAN
Method: calorimetry
Buffer: potassium phosphate (0.15 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

Light is emitted by this reaction.

### 4.19. Enzyme: camphor 5-monooxygenase (EC 1.14.15.1)

(+)-camphor(aq)+NADH(aq)+$O_2$(aq)=(+)-5-*exo*-hydroxycamphor(aq)+NAD(aq)+$H_2O$(l)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 7.4 | −405.8 |

Reference: 69PET/MCK
Method: calorimetry
Buffer: Tris+HCl
pH: 7.4
Evaluation: B

### 4.20. Enzyme: glycine hydroxymethyltransferase (EC 2.1.2.1)

5,10-methylenetetrahydrofolate(aq)+glycine(aq)+$H_2O$(l) =5,6,7,8-tetrahydrofolate(aq)+L-serine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 303.15 | 7.3 | 0.125 |
| 308.15 | 7.5 | 0.083 |

Reference: 77SCH/TAT
Method: spectrophotometry and radioactivity

Buffer: potassium phosphate
pH: 7.3–7.5
Evaluation: A

5,10-methylenetetrahydrofolate(aq)+glycine(aq)+$H_2O$(l) =5,6,7,8-tetrahydrofolate(aq)+L-serine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 7.4 | 0.067 |

Reference: 93BES/REB
Method: radioactivity
Buffer: $KH_2PO_4$ (0.020 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

tetraglutamyl-5,10-methylenetetrahydrofolate(aq) +glycine(aq)+$H_2O$(l)=tetraglutamyl-5,6,7,8-tetrahydrofolate(aq)+L-serine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 7.4 | 0.063 |

Reference: 93BES/REB
Method: radioactivity
Buffer: $KH_2PO_4$ (0.020 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

### 4.21. Enzyme: serine *O*-acetyltransferase (EC 2.3.1.30)

acetyl-CoA(aq)+L-serine(aq)=CoA(aq)+*O*-acetyl-L-serine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 6.0 | 15 |

Reference: 94LEU/COO
Method: spectrophotometry
Buffer: Mes (0.1 mol dm$^{-3}$)
pH: 6.0
Evaluation: A

### 4.22. Enzyme: sucrose synthase (EC 2.4.1.13)

UDPglucose(aq)+D-fructose(aq)=UDP(aq)+sucrose(aq)

| $T$/K | pH | Buffer | $K'$ |
|---|---|---|---|
| 303.15 | 7.0 | Hepes | 6.7 |
| 303.15 | 9.4 | Ches | 250 |

Reference: 97DEJ/ROC
Method: enzymatic assay and spectrophotometry
Buffer: {Hepes (0.050 mol dm$^{-3}$)+NaOH} and {Ches (0.050 mol dm$^{-3}$)+NaOH}
pH: 7.0–9.4
Cofactor(s): $MgCl_2$
Evaluation: B

### 4.23. Enzyme: cyclomaltodextrin glucanotransferase (EC 2.4.1.19)

$G_u$(aq)=cyclomaltohexaose(aq)+$G_{(u-6)}$(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 311.15 | 6.5 | 0.0134 |

Reference: 50PAZ
Method: HPLC
Buffer: NaCN+$NaC_2H_3O_2$
pH: 6.5
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $u$ is an integer $\geqslant 7$. The result given here is based upon Tewari and Goldberg's recalculation [97TEW/GOL] of Pazur's original data.

$G_u$(aq)=cyclomaltohexaose(aq)+$G_{(u-6)}$(aq)

| $T$/K | pH | $K'_m$ |
|---|---|---|
| 329.6 | 5.55 | 0.0229 |

Reference: 97TEW/GOL
Method: HPLC
Buffer: phosphate
pH: 5.55
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $u$ is an integer $\geqslant 7$.

$G_v$(aq)=cyclomaltoheptaose(aq)+$G_{(v-7)}$(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 311.15 | 6.5 | 0.0334 |

Reference: 50PAZ
Method: HPLC
Buffer: NaCN+$NaC_2H_3O_2$
pH: 6.5
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $v$ is an integer $\geqslant 8$. The result given here is based upon Tewari and Goldberg's recalculation [97TEW/GOL] of Pazur's original data.

$G_v$(aq)=cyclomaltoheptaose(aq)+$G_{(v-7)}$(aq)

| $T$/K | pH | $K'_m$ |
|---|---|---|
| 329.6 | 5.55 | 0.0390 |

Reference: 97TEW/GOL
Method: HPLC
Buffer: phosphate
pH: 5.55
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $v$ is an integer $\geq 8$.

$G_w(aq) = cyclomaltooctaose(aq) + G_{(w-8)}(aq)$

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 311.15 | 6.5 | 0.0194 |

Reference: 50PAZ
Method: HPLC
Buffer: $NaCN + NaC_2H_3O_2$
pH: 6.5
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $w$ is an integer $\geq 9$. The result given here is based upon Tewari and Goldberg's recalculation [97TEW/GOL] of Pazur's original data.

$G_w(aq) = cyclomaltooctaose(aq) + G_{(w-8)}(aq)$

| $T$/K | pH | $K'_m$ |
|---|---|---|
| 329.6 | 5.55 | 0.0103 |

Reference: 97TEW/GOL
Method: HPLC
Buffer: phosphate
pH: 5.55
Evaluation: A

$G_1$ represents D-glucose and $G_n$ ($n$ is a positive integer) represents a linear maltodextrin; $w$ is an integer $\geq 9$.

cyclomaltohexaose(aq) + 6 $H_2O$(l) = 6 D-glucose(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 4.58 | −50.85 |

Reference: 97TEW/GOL
Method: calorimetry
Buffer: $KH_2PO_4$ (0.10 mol kg$^{-1}$)
pH: 4.58
Evaluation: A

Glucan1,4-$\alpha$-glucosidase (EC 3.2.1.3) was also present.

## 4.24. Enzyme: cellobiose phosphorylase (EC 2.4.1.20)

cellobiose(aq) + orthophosphate(aq) = D-glucose(aq) + $\alpha$-D-glucose 1-phosphate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 7.0 | 0.23 |

Reference: 61ALE
Method: enzymatic assay
Buffer: barbital (0.0075 mol dm$^{-3}$) + acetate
pH: 7.0
Evaluation: B

## 4.25. Enzyme: UDP-*N*-acetylglucosamine 1-carboxyvinyltransferase (EC 2.5.1.7)

*(Z)*-phospho*enol*butyrate(aq) + UDP-*N*-acetyl-D-glucosamine(aq) = orthophosphate(aq) + *(Z)-enol*butyryl-UDP-*N*-acetylglucosamine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.0 | 65 |

Reference: 95LEE/WAL
Method: HPLC
Buffer: Tris (0.050 mol dm$^{-3}$)
pH: 8.0
Evaluation: C

This is an approximate result.

## 4.26. Enzyme: glutathione transferase (EC 2.5.1.18)

reduced glutathione(aq) + ethyl-(*E*)-2-octenoate(aq) = glutathionyl-ethyl-(*E*)-2-octenoate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.4 | 435 |

Reference: 94CHI/KIR
Method: HPLC
Buffer: phosphate (0.066 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

reduced glutathione(aq) + methyl-(*E*)-2-octenoate(aq) = glutathionyl-methyl-(*E*)-2-octenoate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.4 | 212 |

Reference: 94CHI/KIR
Method: HPLC
Buffer: phosphate (0.066 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

reduced glutathione(aq) + (*E*)-3-nonen-2-one(aq) = glutathionyl-(*E*)-3-nonen-2-one(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.4 | $2.6 \cdot 10^3$ |

Reference: 94CHI/KIR
Method: HPLC

Buffer: phosphate (0.066 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

reduced glutathione(aq) + (*E*) - 2 -octenal(aq) = glutathionyl-(*E*)- 2-octenal(aq)

| *T*/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.4 | $7.1 \cdot 10^3$ |

Reference: 94CHI/KIR
Method: HPLC
Buffer: phosphate (0.066 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

reduced glutathione(aq) + (*E*) - 4 - phenyl - 3-buten-2-one(aq) =4-(glutathionyl)-4-phenyl-2-butanone(aq)

| *T*/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 8.0 | 640 |

Reference: 95CHE/ARM
Method: spectrophotometry
Buffer: Tris (0.1 mol dm$^{-3}$)
pH: 8.0
Evaluation: B

4-(glutathionyl)-4-phenyl-2-butanone) is an equimolar mixture of the (4*R*) and (4*S*) stereoisomers. The sums of the concentrations of the two stereoisomers was used in the calculation of the value of $K'_c$ which was obtained from the analysis of kinetic data.

### 4.27. Enzyme: aspartate transaminase (EC 2.6.1.1)

L-aspartate(aq)+2-oxoglutarate(aq)=oxaloacetate(aq) +L-glutamate(aq)

| | | $I_m$ | |
|---|---|---|---|
| *T*/K | pH | mol·kg$^{-1}$ | *K'* |
| 283.15 | 7.00 | 0.163 | 0.133 |
| 288.15 | 7.12 | 0.167 | 0.144 |
| 292.65 | 7.07 | 0.165 | 0.133 |
| 298.15 | 7.13 | 0.164 | 0.143 |
| 303.15 | 6.94 | 0.163 | 0.145 |

Reference: 98KIS/TEW2
Method: HPLC
Buffer: phosphate
pH: 6.94–7.13
Evaluation: A

Kishore *et al.* calculated $K=0.143$, $\Delta_r H° = 1.9$ kJ mol$^{-1}$, and $\Delta_r S° = -10$ J K$^{-1}$ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-aspartate$^-$(aq)+2-oxoglutarate$^{2-}$(aq)=oxaloacetate$^{2-}$(aq)+L-glutamate$^-$(aq).

### 4.28. Enzyme: alanine transaminase (EC 2.6.1.2)

L-alanine(aq)+2-oxoglutarate(aq)=pyruvate(aq) +L-glutamate(aq)

| | | $I_c$ | |
|---|---|---|---|
| *T*/K | pH | mol·dm$^{-3}$ | *K'* |
| 311.15 | 7.0 | 0.25 | 0.68 |

Reference: 68BRO
Method: spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 7.0
Evaluation: A

Also see Brosnan *et al.* [70BRO/KRE].

L-alanine(aq)+2-oxoglutarate(aq)=pyruvate(aq) +L-glutamate(aq)

| | | $I_c$ | |
|---|---|---|---|
| *T*/K | pH | mol·dm$^{-3}$ | *K'* |
| 311.15 | 7.0 | 0.25 | 0.68 |

Reference: 70BRO/KRE
Method: spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 7.0
Evaluation: A

Also see Brosnan [68BRO].

L-alanine(aq)+2-oxoglutarate(aq)=pyruvate(aq) +L-glutamate(aq)

| | | $I_m$ | |
|---|---|---|---|
| *T*/K | pH | mol·kg$^{-1}$ | *K'* |
| 298.15 | 6.60 | 0.15 | 0.72 |
| 298.15 | 7.23 | 0.19 | 0.78 |

Reference: 98TEW/KIS
Method: HPLC
Buffer: phosphate
pH: 6.60–7.23
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=1.36$ and $\Delta_r H° = 5.9$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-alanine(aq)+2-oxoglutarate$^{2-}$(aq)=pyruvate$^-$(aq) +L-glutamate$^-$(aq).

L-alanine(aq)+2-oxoglutarate(aq)=pyruvate(aq) +L-glutamate(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| *T*/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.37 | 0.34 | 5.2 |

Reference: 98TEW/KIS
Method: calorimetry
Buffer: phosphate
pH: 7.37
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=1.36$ and $\Delta_r H°=5.9$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-alanine(aq)+2-oxoglutarate$^{2-}$(aq)=pyruvate$^-$(aq)+L-glutamate$^-$(aq).

### 4.29. Enzyme: tyrosine transaminase (EC 2.6.1.5)

L-phenylalanine(aq)+2-oxoglutarate(aq)=phenylpyruvate(aq)+L-glutamate(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'$ |
| 298.15 | 7.46 | 0.32 | 1.024 |
| 298.15 | 7.57 | 0.33 | 1.069 |

Reference: 98TEW/KIS
Method: HPLC
Buffer: phosphate
pH: 7.46–7.57
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=2.14$ and $\Delta_r H°=9.5$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-phenylalanine(aq)+2-oxoglutarate$^{2-}$(aq)=phenylpyruvate$^-$(aq)+L-glutamate$^-$(aq).

L-phenylalanine(aq)+2-oxoglutarate(aq)=phenylpyruvate(aq)+L-glutamate(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.30 | 0.34 | 8.3 |

Reference: 98TEW/KIS
Method: calorimetry
Buffer: phosphate
pH: 7.30
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=2.14$ and $\Delta_r H°=9.5$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-phenylalanine(aq)+2-oxoglutarate$^{2-}$(aq)=phenylpyruvate$^-$(aq)+L-glutamate$^-$(aq).

L-tyrosine(aq)+2-oxoglutarate(aq)=4-hydroxyphenylpyruvate(aq)+L-glutamate(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'$ |
| 298.15 | 7.45 | 0.32 | 0.880 |
| 298.15 | 7.74 | 0.33 | 0.876 |

Reference: 98TEW/KIS
Method: HPLC
Buffer: phosphate
pH: 7.45–7.74
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=1.82$ and $\Delta_r H°=10.1$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-tyrosine(aq)+2-oxoglutarate$^{2-}$(aq)=4-hydroxyphenylpyruvate$^-$(aq)+L-glutamate$^-$(aq).

L-tyrosine(aq)+2-oxoglutarate(aq)=4-hydroxyphenylpyruvate(aq)+L-glutamate(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.64 | 0.34 | 8.4 |

Reference: 98TEW/KIS
Method: calorimetry
Buffer: phosphate
pH: 7.64
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=1.82$ and $\Delta_r H°=10.1$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: L-tyrosine(aq)+2-oxoglutarate$^{2-}$(aq)=4-hydroxyphenylpyruvate$^-$(aq)+L-glutamate$^-$(aq).

### 4.30. Enzyme: branched-chain-amino-acid transaminase (EC 2.6.1.42)

L-leucine(aq)+2-oxoglutarate(aq)=4-methyl-2-oxopentanoate(aq)+L-glutamate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 8.6 | 1.75 |

Reference: 70JEN/TAY
Method: spectrophotometry
Buffer: Tris
pH: 8.6
Evaluation: C

Few details are given in this study.

### 4.31. Enzyme: polyamine transaminase (EC 2.6.1.-)

L-alanine(aq)+3-aminopropionaldehyde(aq)=pyruvate(aq)+1,3-diaminopropane(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 303.15 | 9.0 | 2.9 |

Reference: 97YOR/ISH
Method: spectrophotometry

Buffer: Tris (0.1 mol dm$^{-3}$) + HCl
pH: 9.0
Evaluation: B

### 4.32. Enzyme: choline kinase (2.7.1.32)

ATP(aq) + choline(aq) = ADP(aq) + *O*-phosphocholine(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 303.15 | 9.5 | 0.2 |

Reference: 98KIM/VOE
Method: radioactivity
Buffer: glycine (0.067 mol dm$^{-3}$) + NaOH
pH: 9.5
Cofactor(s): $MgSO_4$ (0.010 mol dm$^{-3}$)
Evaluation: B

### 4.33. Enzyme: phosphoglycerate kinase (EC 2.7.2.3)

ATP(aq) + 3-phospho-D-glycerate(aq) = ADP(aq) + 3-phospho-D-glyceroyl phosphate(aq)

| *T*/K | pH | Cosolvent | *K'* |
|---|---|---|---|
| 277.15 | 7.5 | none | 0.000 15 |
| 277.15 | 7.5 | ethylene glycol, 40% | 0.000 08 |

Reference: 95SCH/TRA
Method: radioactivity
Buffer: triethanolamine (0.020 mol dm$^{-3}$)
pH: 7.5
Cofactor(s): $Mg^{2+}$ (0.001 mol dm$^{-3}$)
Evaluation: C

Schmidt *et al.* did not state what the "percent" of ethylene glycol was, i.e., volume percent, mass percent, or mole percent.

### 4.34. Enzyme: creatine kinase (EC 2.7.3.2)

phosphocreatine(aq) + cyclocreatine(aq) = creatine(aq) + phosphocyclocreatine(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 296.15 | 7.0 | 34.3 |

Reference: 95WIS/KUS
Method: NMR and HPLC
Buffer: Mops (0.1 mol dm$^{-3}$) + Tris (0.070 mol dm$^{-3}$)
pH: 7.0
Evaluation: B

phosphocreatine(aq) + β-guanidinopropionate(aq) = creatine(aq) + β-phosphoguanidinopropionate(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 298.15 | 7.06 | 3.06 |

Reference: 86MEY/BRO
Method: enzymatic assay
Buffer: Pipes (0.050 mol dm$^{-3}$)
pH: 7.06
Cofactor(s): $MgCl_2$ (0.010 mol dm$^{-3}$)
Evaluation: B

The temperature was assumed to be 298.15 K.

phosphocreatine(aq) + β-guanidinopropionate(aq) = creatine(aq) + β-phosphoguanidinopropionate(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 296.15 | 7.0 | 3.1 |

Reference: 95WIS/KUS
Method: NMR and HPLC
Buffer: Mops (0.1 mol dm$^{-3}$) + Tris (0.070 mol dm$^{-3}$)
pH: 7.0
Evaluation: B

### 4.35. Enzyme: arginine kinase (2.7.3.3)

ATP(aq) + L-arginine(aq) = ADP(aq) + $N^{\omega}$-phospho-L-arginine(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 298.15 | 7.2 | 17.5 |

Reference: 97CHA
Method: spectrophotometry
Buffer: imidazole (0.1 mol dm$^{-3}$)
pH: 7.2
Cofactor(s): $MgCl_2$ (0.005 mol dm$^{-3}$)
Evaluation: B

### 4.36. Enzyme: taurocyamine kinase (EC 2.7.3.4)

ATP(aq) + taurocyamine(aq) = ADP(aq) + $N^{\omega}$-phosphotaurocyamine(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 285.15 | 7.3 | $1 \cdot 10^9$ |

Reference: 95KAM/JUR
Method: enzymatic analysis
Buffer: Tris (0.1 mol dm$^{-3}$) + HCl
pH: 7.3
Cofactor(s): magnesium acetate (0.10 mol dm$^{-3}$)
Evaluation: C

The reported value of *K'* is exceptionally large and it is not clear how it could have been measured.

### 4.37. Enzyme: adenylate kinase (EC 2.7.4.3)

2 ADP(aq) = AMP(aq) + ATP(aq)

| *T*/K | pH | *K'* |
|---|---|---|
| 285.15 | 7.3 | 0.36 |

Reference: 95KAM/JUR

Method: enzymatic analysis
Buffer: Tris (0.1 mol dm$^{-3}$)+HCl
pH: 7.3
Cofactor(s): magnesium acetate (0.060 mol dm$^{-3}$)
Evaluation: C

### 4.38. Enzyme: guanylate kinase (EC 2.7.4.8)

ATP(aq)+GMP(aq)=ADP(aq)+GDP(aq)

| $T$/K | pH | $c(MgCl_2)$ / mol·dm$^{-3}$ | $K'$ |
|---|---|---|---|
| 298.15 | 7.5 | 0.0056 | 1.5 |
| 298.15 | 7.5 | 0.013 | 3.1 |
| 298.15 | 7.5 | 0.020 | 5.2 |
| 298.15 | 7.5 | 0.045 | 5.3 |
| 298.15 | 7.7 | 0.0050 | 2.1 |

Reference: 96LI/ZHA
Method: NMR and radioactivity
Buffer: Tris+HCl
pH: 7.5–7.7
Cofactor(s): $Mg^{2+}$
Evaluation: A

Results obtained from kinetic experiments were also found to be consistent with the values of $K'$ obtained from the equilibrium measurements.

### 4.39. Enzyme: UTP-glucose-1-phosphate uridylyltransferase (EC 2.7.7.9)

UTP(aq)+$\alpha$-D-glucose 1-phosphate(aq)=pyrophosphate(aq)+UDPglucose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 303.15 | 8.5 | 0.26 |

Reference: 69TSU/FUK
Method: fluorimetry
Buffer: Tris (0.050 mol dm$^{-3}$)
pH: 8.5
Cofactor(s): $MgCl_2$
Evaluation: B

### 4.40. Enzyme: [glutamate-ammonia-ligase] adenylyltransferase (EC 2.7.7.42)

ATP(aq)+[L-glutamate:ammonia ligase (ADP-forming)](aq) = pyrophosphate(aq)+adenylyl-[L-glutamate:ammonia ligase (ADP-forming)](aq)

| $T$/K | pH | Buffer | $c(MgSO_4)$ / mol·dm$^{-3}$ | pMg | $K'$ |
|---|---|---|---|---|---|
| 278.5 | 7.4 | Tris | 0.010 | 2.0 | 57.4 |
| 283.2 | 7.4 | Tris | 0.010 | 2.0 | 28.8 |
| 288.0 | 7.4 | Tris | 0.010 | 2.0 | 21.8 |
| 298.2 | 7.4 | Tris | 0.010 | 2.0 | 19.6 |
| 303.0 | 7.4 | Tris | 0.010 | 2.0 | 17.8 |
| 303.15 | 6.73 | Tris | 0.010 | not given | 5.0 |
| 303.15 | 7.0 | imidazole | 0.010 | not given | 12.9 |
| 303.15 | 7.03 | Tris | 0.010 | not given | 12.8 |
| 303.15 | 7.4 | Tris | 0.0027 | not given | 4.2 |
| 303.15 | 7.4 | Tris | 0.005 | not given | 12.3 |
| 303.15 | 7.4 | Tris | 0.010 | not given | 23.6 |
| 303.15 | 7.4 | Tris | 0.020 | not given | 38.2 |
| 303.15 | 7.57 | Tris | 0.010 | not given | 48.2 |
| 309.5 | 7.4 | Tris | not given | 2.0 | 18.5 |

Reference: 71WOH
Method: enzymatic assay
Buffer: {Tris (0.10 mol dm$^{-3}$)+HCl} and {imidazole (0.1 mol dm$^{-3}$)+HCl}
pH: 6.73–7.57
Evaluation: A

The apparent equilibrium constants given here were obtained from Wohlhueter's Table 3 and Figs. 2, 3, and 4. We calculate $\Delta_r H'^\circ(\langle T\rangle = 291$ K, pH=7.4, pMg=2.0)$\approx -28$ kJ mol$^{-1}$ from the temperature dependency of the apparent equilibrium constant.

### 4.41. Enzyme: UDPhexose synthase (EC 2.7.7.-)

UDPglucose (aq) + imidazole (aq) = $\alpha$-D-glucose 1-phosphate(aq)+UMPimidazole(aq)

| $T$/K | pH | Buffer | $K'$ |
|---|---|---|---|
| 300.15 | 7.0 | MOPS | 0.00064 |
| 300.15 | 8.5 | bicine | 0.022 |

Reference: 96ARA/RUZ
Method: HPLC and fluorimetry
Buffer: Mops (0.095 mol·dm$^{-3}$) and Bicine (0.095 mol·dm$^{-3}$)
pH: 7.0–8.5
Evaluation: A

UDPhexose synthase is a mutant of UDPglucose-hexose-1-phosphate uridylyltransferase (EC 2.7.7.12).

### 4.42. Enzyme: triacylglycerol lipase (EC 3.1.1.3)

1-dodecanoic acid(sln)+1-dodecanol(sln)=dodecyldodecanoate(sln)+$H_2O$(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 298.15 | hexane | 39.6 |
| 298.15 | heptane | 35.3 |
| 298.15 | cyclohexane | 23.3 |
| 298.15 | 2,2,4-trimethylpentane | 27.2 |
| 298.15 | toluene | 17.9 |

Reference: 98TEW
Method: HPLC, GC, and Karl Fischer analysis
Evaluation: A

This reaction was studied in five organic solvents. Tewari also calculated $K_m(T=298.15\ \text{K}, I=0)=2.9\cdot10^6$ for the reaction: 1-dodecanol(aq) + 1-dodecanoic acid(aq) =dodecyldodecanoate(aq)+$H_2O$(l).

1-dodecanoic acid(sln)+(-)-menthol(sln)=(-)-menthyldodecanoate(sln)+$H_2O$(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 298.15 | *n*-hexane | 6.5 |
| 298.15 | *n*-heptane | 21.7 |
| 298.15 | cyclohexane | 23.7 |
| 298.15 | 2,2,4-trimethylpentane | 16.2 |
| 298.15 | toluene | 12.0 |
| 298.15 | acetonitrile | 3.23 |
| 298.15 | 2-methyl-2-butanol | 5.8 |

Reference: 99TEW/SCH
Method: GC and Karl Fischer
Evaluation: A

This reaction was studied in seven organic solvents. Tewari *et al.* also determined saturation molalities and (hexane +$H_2O$) partition coefficients for (-)-menthol, 1-dodecanoic acid, and (-)menthyldodecanoate. By using a thermodynamic cycle calculation they calculated $K_m(T=298.15\ \text{K}, I=0)=1.9\cdot10^5$ for the reference reaction: (-)-menthol(aq) +1-dodecanoic acid(aq)=(-)-menthyl dodecanoate(aq) +$H_2O$(l).

tributyrylglycerol(sln) + (*R*)-2-decanol(sln) = (*R*)-2-decyl-butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 303.15 | hexane | 0.015 |
| 303.15 | benzene | 0.018 |
| 303.15 | dioxane | 0.025 |
| 303.15 | acetonitrile | 0.028 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

tributyrylglycerol(sln)+(*R*)-2-dodecanol(sln)=(*R*)-2-dodecyl butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 303.15 | hexane | 0.017 |
| 303.15 | benzene | 0.017 |
| 303.15 | dioxane | 0.020 |
| 303.15 | acetonitrile | 0.025 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

tributyrylglycerol(sln)+(*R*)-2-heptanol(sln)=(*R*)-2-heptyl butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 303.15 | hexane | 0.026 |
| 303.15 | benzene | 0.028 |
| 303.15 | dioxane | 0.037 |
| 303.15 | acetonitrile | 0.038 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

tributyrylglycerol(sln)+(*R*)-2-nonanol(sln)=(*R*)-2-nonyl butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 303.15 | hexane | 0.020 |
| 303.15 | benzene | 0.020 |
| 303.15 | dioxane | 0.027 |
| 303.15 | acetonitrile | 0.029 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

tributyrylglycerol(sln)+(*R*)-2-octanol(sln)=(*R*)-2-octyl butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 303.15 | hexane | 0.022 |
| 303.15 | benzene | 0.024 |
| 303.15 | dioxane | 0.028 |
| 303.15 | acetonitrile | 0.029 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

tributyrylglycerol(sln)+(*R*)-2-undecanol(sln)=(*R*)-2-undecyl butyrate(sln)+glycerol-1,2-dibutyrate(sln)

| *T*/K | Solvent | *K* |
|---|---|---|
| 303.15 | hexane | 0.017 |
| 303.15 | benzene | 0.017 |
| 303.15 | dioxane | 0.022 |
| 303.15 | acetonitrile | 0.026 |

Reference: 96HIR/MAY
Method: HPLC and GC
Evaluation: B

The results obtained with hexane and benzene are the averages of the results obtained using two different lipases.

### 4.43. Enzyme: tannase (EC 3.1.1.20)

3,4,5-trihydroxybenzoic acid propyl ester(aq)+$H_2O$(l)=3,4,5-trihydroxybenzoate(aq)+1-propanol(aq)

| *T*/K | *p*H | $I_m$ / mol·kg$^{-1}$ | $K'_m$ |
|---|---|---|---|
| 293.15 | 5.33 | 0.080 | 126 |
| 293.15 | 5.31 | 0.080 | 119 |
| 298.15 | 4.99 | 0.052 | 57.3 |
| 298.15 | 5.00 | 0.052 | 61.1 |
| 298.15 | 5.32 | 0.080 | 122.1 |
| 298.15 | 5.36 | 0.082 | 117 |
| 298.15 | 5.38 | 0.084 | 147 |
| 298.15 | 5.39 | 0.085 | 128 |
| 298.15 | 5.91 | 0.109 | 435 |
| 298.15 | 5.91 | 0.111 | 448 |
| 298.15 | 6.56 | 0.135 | 2409 |
| 298.15 | 6.56 | 0.135 | 2820 |
| 303.15 | 5.37 | 0.082 | 121 |
| 303.15 | 5.35 | 0.081 | 123 |
| 308.15 | 5.32 | 0.081 | 114 |
| 308.15 | 5.34 | 0.081 | 124 |

Reference: 96TEW/SCH
Method: HPLC
Buffer: sodium acetate
*p*H: 4.99–6.56
Evaluation: A

Tewari *et al.* also calculated $K_m=4.37\cdot10^{-4}$ and $\Delta_rH°=-4.6$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: 3,4,5-trihydroxybenzoic acid propyl ester(aq)+$H_2O$(l)=3,4,5-trihydroxybenzoate$^-$(aq)+1-propanol(aq)+$H^+$(aq).

3,4,5-trihydroxybenzoic acid propyl ester(aq)+$H_2O$(l)=3,4,5-trihydroxybenzoate(aq)+1-propanol(aq)

| *T*/K | pH | Buffer | $I_m$ / mol·kg$^{-1}$ | $\Delta_rH$(cal) / kJ·mol$^{-1}$ |
|---|---|---|---|---|
| 298.15 | 5.61 | phosphate | 0.092 | −8.33 |
| 298.15 | 6.18 | Mes | 0.027 | −19.8 |

Reference: 96TEW/SCH
Method: HPLC
Buffer: phosphate and Mes
pH: 5.61–6.18
Evaluation: A

Tewari *et al.* also calculated $K_m=4.37\cdot10^{-10}$ and $\Delta_rH°=-4.6$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: 3,4,5-trihydroxybenzoic acid propyl ester(aq)+$H_2O$(l)=3,4,5-trihydroxybenzoate$^-$(aq)+1-propanol(aq)+$H^+$(aq).

3,4,5-trihydroxybenzoic acid propyl ester(sln)+$H_2O$(sln)=3,4,5-trihydroxybenzoate(sln)+1-propanol(sln)

| *T*/K | *K* |
|---|---|
| 293.25 | 0.0128 |
| 298.25 | 0.0130 |
| 303.15 | 0.0112 |
| 308.15 | 0.0098 |

Reference: 96TEW/SCH
Method: HPLC, GC, and Karl Fischer analysis
Evaluation: A

Toluene was the solvent used in this study. Tewari *et al.* also calculated $\Delta_rH°(\langle T\rangle=301\text{ K})=-15.4$ kJ mol$^{-1}$ from the temperature dependence of the equilibrium constant.

### 4.44. Enzyme: pancreatic ribonuclease (3.1.27.5)

guanosine 2′:3′-(cyclic)phosphate(aq)+$H_2O$(l)=guanosine 3′-monophosphate(aq)

| *T*/K | pH | *K′* |
|---|---|---|
| 308.15 | 6.0 | ≈13 |

Reference: 98LOV/LAU
Method: mass spectrometry
Buffer: imidazole (0.0125 mol dm$^{-3}$)
pH: 6.0
Evaluation: B

Ribonuclease T1 (EC 3.1.27.3) was also used in this study. The value of $K'$ given here was calculated from the average value $K'c°/c(H_2O)=0.38$ given by Loverix *et al.* in their Table 1. The solution used in this study contained methanol

(40% by volume). This result is based on the analysis of kinetic data.

guanosine 2′ : 3′ - (cyclic) phosphate (aq) + methanol (aq) =guanosine 3′-methylphosphate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 308.15 | 6.0 | ≈0.95 |

Reference: 98LOV/LAU
Method: mass spectrometry
Buffer: imidazole (0.0125mol $dm^{-3}$)
pH: 6.0
Evaluation: B

Ribonuclease T1 (EC 3.1.27.3) was also used. This result is based on the analysis of kinetic data.

uridine 2′: 3′ - (cyclic)phosphate(aq)+$H_2O$(l) = uridine 3′-monophosphate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 5.0 | 440 |

Reference: 69ROS/HAM
Method: chromatography and radioactivity
Buffer: Tris (0.1 mol $dm^{-3}$) + acetate
pH: 5.0
Evaluation: B

### 4.45. Enzyme: α-amylase (EC 3.2.1.1)

cyclomaltoheptaose(aq)+7 $H_2O$(l)=7 D-glucose(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·$mol^{-1}$ |
| 298.15 | 5.14 | −48.79 |

Reference: 97TEW/GOL
Method: calorimetry
Buffer: $KH_2PO_4$ (0.10 mol $kg^{-1}$)
pH: 5.14
Evaluation: A

Glucan 1,4-α-glucosidase (EC 3.2.1.3) was also present.

cyclomaltooctaose(aq)+8 $H_2O$(l)=8 D-glucose(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·$mol^{-1}$ |
| 298.15 | 5.15 | −52.29 |

Reference: 97TEW/GOL
Method: calorimetry
Buffer: $KH_2PO_4$ (0.10 mol $kg^{-1}$)
pH: 5.15
Evaluation: A

Glucan 1,4-α-glucosidase (EC 3.2.1.3) was also present.

### 4.46. Enzyme: glucan 1,4-α-glucosidase (EC 3.2.1.3)

6-*O*-α-D-galactopyranosyl-D-galactopyranose(aq) +$H_2O$(l)=2 D-galactose(aq)

| $T$/K | $p$H | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | ≈$1.04 \cdot 10^3$ |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol $dm^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table V. In this study, the position of equilibrium was not approached from both directions. Pestlin *et al.* also report additional data for reactions where the exact identity of the products is uncertain.

4-*O*-α-D-glucopyranosyl-D-fructofuranose(aq)+$H_2O$(l) =D-glucose(aq)+D-fructose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 372 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol $dm^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table IV.

3-*O*-α-D-glucopyranosyl-lyxopyranose(aq)+$H_2O$(l) =D-glucose(aq)+lyxose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 330 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol $dm^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VII.

α-isomaltose(aq)+$H_2O$(l)=2 D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 81 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here is the average of the results calculated from the concentrations given in Pestlin *et al.*'s Tables III to X.

$\beta$-isomaltose(aq)+$H_2O$(l)=2 D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 65 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here is the average of the results calculated from the concentrations given in Pestlin *et al.*'s Tables III to X.

1-*O*-$\alpha$-D-mannopyranosyl-D-mannofuranose(aq)+$H_2O$(l) =2 D-mannose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | $1.26 \cdot 10^3$ |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VIII.

6-*O*-$\alpha$-D-mannopyranose-D-mannopyranose(aq)+$H_2O$(l) =2 D-mannose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | ≈420 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VIII.

$\alpha$-D-melibiose(aq)+$H_2O$(l)=D-galactose(aq) +D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 53 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table V.

$\beta$-D-melibiose(aq)+$H_2O$(l)=D-galactose(aq) +D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 318.15 | 4.5 | 40 |

Reference: 97PES/PRI
Method: GC+MS
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.5
Evaluation: B

The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table V.

### 4.47. Enzyme: $\beta$-galactosidase (EC 3.2.1.23)

*allo*lactose(aq)+$H_2O$(l)=D-galactose(aq)+D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.0 | 45 |

Reference: 92ELL/SRI
Method: HPLC
Buffer: Tes (0.030 mol dm$^{-3}$)+NaOH
pH: 7.0
Cofactor(s): $MgCl_2$(0.001 mol dm$^{-3}$)
Evaluation: A

lactose(aq)+$H_2O$(l)=D-galactose(aq)+D-glucose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.0 | 152 |

Reference: 92ELL/SRI
Method: HPLC
Buffer: Tes (0.030 mol dm$^{-3}$)+NaOH
pH: 7.0
Cofactor(s): $MgCl_2$(0.001 mol dm$^{-3}$)
Evaluation: A

lactulose(aq)+$H_2O$(l)=D-galactose(aq)+D-fructose(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.0 | 40 |

Reference: 92ELL/SRI
Method: HPLC

Buffer: Tes (0.030 mol dm$^{-3}$)+NaOH
pH: 7.0
Cofactor(s): $MgCl_2$(0.001 mol dm$^{-3}$)
Evaluation: A

### 4.48. Enzyme: β-fructofuranosidase (EC: 3.2.1.26)

sucrose(aq)+$H_2O$(l)=D-glucose(aq)+D-fructose(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 4.6 | −15.5 |

Reference: 99HUT/OEH
Method: calorimetry
Buffer: acetate (0.05 mol dm$^{-3}$)
pH: 4.6
Cofactor(s): $Cd^{2+}$, $Zn^{2+}$, $As^{3+}$, $As^{+5}$, and $Ag^{+}$
Evaluation: B

The result given here is the average of the results obtained from experiments in which several different heavy metal ion cofactors were present. This result is in agreement with the result obtained from experiments in which no heavy metal ions were present.

### 4.49. Enzyme: chymotrypsin (EC 3.4.21.1)

*N*-acetyl-L-phenylalanine ethyl ester(aq)+$H_2O$(l)
=*N*-acetyl-L-phenylalanine(aq)+ethanol(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'_m$ |
| 288.15 | 6.09 | 0.11 | $3.55\cdot10^3$ |
| 288.15 | 6.29 | 0.11 | $7.98\cdot10^3$ |
| 293.15 | 6.17 | 0.11 | $2.27\cdot10^3$ |
| 293.15 | 6.39 | 0.13 | $4.28\cdot10^3$ |
| 298.15 | 6.19 | 0.12 | $4.04\cdot10^3$ |
| 298.15 | 6.44 | 0.13 | $5.29\cdot10^3$ |
| 308.15 | 5.98 | 0.11 | $1.63\cdot10^3$ |
| 308.15 | 6.23 | 0.12 | $1.99\cdot10^3$ |

Reference: 95TEW/SCH
Method: HPLC and GC
Buffer: phosphate
pH: 5.98–6.44
Evaluation: A

Tewari *et al.* also calculated $K_m=1.7\cdot10^{-3}$ and $\Delta_r H°=-3.5$ kJ mol$^{-1}$ at $T=298.15$ K and $I=0$ for the reference reaction: *N*-acetyl-L-phenylalanine ethyl ester(aq)+$H_2O$(l) =*N*-acetyl-L-phenylalanine$^-$(aq)+ethanol(aq)+$H^+$(aq).

*N*-acetyl-L-phenylalanine ethyl ester(sln)+$H_2O$(sln)
=*N*-acetyl-L-phenylalanine(sln)+ethanol(sln)

| $T$/K | Solvent | $K$ |
|---|---|---|
| 283.15 | dichloromethane | 0.0377 |
| 288.15 | dichloromethane | 0.0437 |
| 293.25 | dichloromethane | 0.0513 |
| 298.25 | dichloromethane | 0.0572 |
| 283.15 | carbon tetrachloride | 0.38 |
| 288.15 | carbon tetrachloride | 0.30 |
| 293.25 | carbon tetrachloride | 0.23 |
| 298.25 | carbon tetrachloride | 0.197 |
| 283.15 | toluene | 0.182 |
| 288.15 | toluene | 0.201 |
| 293.25 | toluene | 0.144 |
| 298.25 | toluene | 0.107 |

Reference: 95TEW/SCH
Method: HPLC, GC, and Karl Fischer analysis
Evaluation: A

Tewari *et al.* calculated the following values of $\Delta_r H°$ from the temperature dependence of the equilibrium constants: $\Delta_r H°(\langle T\rangle=291\text{ K})=20$ kJ mol$^{-1}$ for the reaction in dichloromethane; $\Delta_r H°(\langle T\rangle=291\text{ K})=-28$ kJ mol$^{-1}$ for the reaction in carbon tetrachloride; and $\Delta_r H°(\langle T\rangle=291\text{ K})=-26$ kJ mol$^{-1}$ for the reaction in toluene.

*N*-acetyl-L-tryptophan ethyl ester(aq)+$H_2O$(l)=*N*-acetyl-L-tryptophan(aq)+ethanol(aq)

| | | $I_c$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·dm$^{-3}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.5 | 0.1 | −5.9 |

Reference: 71RAJ/LUM
Method: calorimetry
Buffer: phosphate (0.05 mol dm$^{-3}$)
pH: 7.5
Evaluation: B

Rajender *et al.* applied buffer protonation and ionization corrections to obtain $\Delta_r H°=3.3$ kJ mol$^{-1}$ for the reference reaction: *N*-acetyl-L-tryptophan ethyl ester(aq)+$H_2O$(l)=*N*-acetyl-L-tryptophan(aq)+ethanol(aq).

*N*-acetyl-L-tyrosine ethyl ester(aq)+$H_2O$(l)=*N*-acetyl-L-tyrosine(aq)+ethanol(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ mol$^{-1}$ |
| 298.15 | 7.8 | −48.5 |

Reference: 95LIU/ZEN
Method: calorimetry
Buffer: Tris

pH: 7.8
Evaluation: B

2-propylhippurate(aq) + $H_2O$(l) = 2-propanol(aq) + hippurate(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ mol$^{-1}$ |
|---|---|---|
| 298.15 | 7.0 | −48.9 |

Reference: 95LIU/ZEN
Method: calorimetry
Buffer: Tris
pH: 7.0
Evaluation: B

### 4.50. Enzyme: thermolysin (EC 3.4.24.27)

*N*-(benzyloxycarbonyl)-L-aspartyl-L-phenylalanine methyl ester(aq) + $H_2O$(l) = *N*-(benzyloxycarbonyl)-L-aspartic acid(aq) + L-phenylalanine methyl ester(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 313.15 | 6.0 | 0.79 |

Reference: 86NAK/KIM
Method: HPLC
Buffer: Mes (0.05 M) + NaOH
pH: 6.0
Cofactor(s): $CaCl_2$ (0.005 mol dm$^{-3}$)
Evaluation: B

Nakanishi *et al.* reported $K'_c \cdot c(H_2O) = 1/70$. The apparent equilibrium constant given here was calculated from this result.

*N*-(benzyloxycarbonyl)-L-aspartyl-L-phenylalanine methyl ester(aq) + $H_2O$(l) = *N*-(benzyloxycarbonyl)-L-aspartic acid(aq) + L-phenylalanine methyl ester(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 313.15 | ≈6.5 | 0.67 |

Reference: 84OYA/IRI
Method: HPLC
Buffer: No specific buffering system was used. The pH was adjusted with NaOH.
pH: ≈6.5
Evaluation: B

### 4.51. Enzyme: asparaginase (EC 3.5.1.1)

L-asparagine(aq) + $H_2O$(l) = L-aspartate(aq) + ammonia(aq)

| $T$/K | pH | $I_m$ mol·kg$^{-1}$ | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 7.03 | 0.27 | −25.63 |

Reference: 99KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 7.03
Evaluation: A

Kishore *et al.* also calculated $\Delta_r H°(T = 298.15\ \text{K}, I = 0) = -26.2\ \text{kJ mol}^{-1}$ for the reference reaction: L-asparagine$^{\pm}$(aq) + $H_2O$(l) = L-aspartate$^-$(aq) + $NH_4^+$(aq).

### 4.52. Enzyme: glutaminase (EC 3.5.1.2)

L-glutamine(aq) + $H_2O$(l) = L-glutamate(aq) + ammonia(aq)

| $T$/K | pH | $I_m$ mol·kg$^{-1}$ | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 5.14 | 0.11 | −24.39 |

Reference: 99KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 5.14
Evaluation: A

Kishore *et al.* also calculated $\Delta_r H°(T = 298.15\ \text{K}, I = 0) = -25.2\ \text{kJ mol}^{-1}$ for the reference reaction: L-glutamine$^{\pm}$(aq) + $H_2O$(l) = L-glutamate$^-$(aq) + $NH_4^+$(aq).

### 4.53. Enzyme: urease (EC 3.5.1.5)

ammonium carbamate(aq) + $H_2O$(l) = 2 ammonia(aq) + carbon dioxide(aq)

| $T$/K | pH | Buffer | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 6.3 | Mes | −18.2 |
| 298.15 | 6.86 | phosphate | −32.7 |
| 298.15 | 7.0 | Hepes | −14.7 |
| 298.15 | 8.0 | Tris | 8.7 |

Reference: 95HUT/BOH
Method: calorimetry
Buffer: phosphate, Tris, Mes, and Hepes
pH: 6.86–8.0
Evaluation: B

urea(aq) + 2 $H_2O$(l) = 2 ammonia(aq) + carbon dioxide(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 300.15 | 7.0 | −7.1 |
| 300.15 | 8.0 | −8.4 |

Reference: 76SCH/KRI

Method: calorimetry
Buffer: Tris (0.05 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

urea(aq)+2 $H_2O$(l)=2 ammonia(aq)+carbon dioxide(aq)

| $T$/K | pH | Buffer | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 6.0 | phosphate | −52.9 |
| 298.15 | 6.5 | phosphate | −61.0 |
| 298.15 | 6.86 | phosphate | −58.6 |
| 298.15 | 7.6 | phosphate | −50.9 |
| 298.15 | 7.0 | Tris | −16.4 |
| 298.15 | 6.3 | Mes | −46.0 |
| 298.15 | 7.0 | Hepes | −42.0 |

Reference: 95HUT/BOH
Buffer: phosphate, Tris, Mes, and Hepes
pH: 6.0–7.6
Evaluation: B

urea(aq)+2 $H_2O$(l)=2 ammonia(aq)+carbon dioxide(aq)

| $T$/K | pH | $I_c$ mol·dm$^{-3}$ | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 7.0 | 0.07 | −59.6 |

Reference: 95JUS/KOT
Method: calorimetry
Buffer: phosphate (0.022 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

### 4.54. Enzyme: penicillin amidase (EC 3.5.1.11)

amoxicillin(aq)+$H_2O$(l)=6-aminopenicillanic acid(aq)
+D-4-hydroxyphenylglycine(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 5.0 | 2.86 |
| 298.15 | 5.6 | 7.04 |
| 298.15 | 6.0 | 17.7 |

Reference: 98DIE/STR
Method: HPLC
Buffer: $K_2HPO_4$ (0.1 mol dm$^{-3}$)+NaOH or HCl
pH: 5.0–6.0
Evaluation: A

The values of $K'_c$ given here were obtained from Diender *et al.*'s Fig. 3. Diender *et al.* also report values of the pKs and solubilities of the reactants and products.

### 4.55. Enzyme: aminoacylase (EC 3.5.1.14)

*N*-acetyl-L-methionine(aq)+$H_2O$(l)=L-methionine(aq)
+acetate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.0 | 2.7 |

Reference: 95BIS/KRA
pH: 7.0
Evaluation: C

Few details are given in this study.

### 4.56. Enzyme: D-(-)-phenylglycyl-β-lactamide amidohydrolase (EC 3.5.1.-)

ampicillin(aq)+$H_2O$(l)=6-aminopenicillanic acid(aq)
+D(-)-α-aminophenylacetic acid(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 5.50 | 0.18 |

Reference: 93BLI/MAR
pH: 5.50
Evaluation: B

cephalexin(aq) + $H_2O$(l) = 7-aminodeacetoxycephalosporanic acid(aq)+D(-)-α-aminophenylacetic acid(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 5.25 | 0.12 |

Reference: 93BLI/MAR
pH: 5.25
Evaluation: B

### 4.57. Enzyme: arginase (EC 3.5.3.1)

L-arginine(aq)+$H_2O$(l)=L-ornithine(aq)+urea(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 9.4 | −17.8 |

Reference: 95LIA/WAN2
Method: calorimetry
Buffer: diethylbarbiturate
pH: 9.4
Evaluation: B

This same result was also given later by Liang *et al.* [96LIA/WAN].

L-arginine(aq)+$H_2O(l)$=L-ornithine(aq)+urea(aq)

| $T$/K | pH | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|
| 298.15 | 9.5 | −18.1 |

Reference: 95LIU/ZEN
Method: calorimetry
Buffer: glycine+NaOH
pH: 9.5
Evaluation: B

### 4.58. Enzyme: *N*-acetylneuraminate lyase (EC 4.1.3.3)

N-acetylneuraminate(aq) = *N*-acetyl-D-mannosamine(aq) +pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.2 | 0.096 |

Reference: 62BRU/JOU
Method: radioactivity and spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 7.2
Evaluation: A

This result supersedes the earlier result of Comb and Roseman [62COM/ROS].

N-acetylneuraminate(aq) = *N*-acetyl-D-mannosamine(aq) +pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.7 | 0.08 |

Reference: 84UCH/TSU
Method: spectrophotometry
Buffer: phosphate (0.050 mol dm$^{-3}$)
pH: 7.7
Evaluation: B

The apparent equilibrium constant given here was calculated from the data given in Uchida *et al.*'s Fig. 7.

N-acetylneuraminate(aq) = *N*-acetyl-D-mannosamine(aq) +pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 283.15 | 7.5 | 0.0120 |
| 298.15 | 7.5 | 0.0348 |

Reference: 91KRA/GYG
Method: HPLC
Buffer: none
pH: 7.5
Evaluation: A

Also see Kragel's thesis [92KRA].

N-acetylneuraminate(aq)=*N*-acetyl-D-mannosamine(aq) +pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 278.3 | 7.5 | 0.00898 |
| 287.9 | 7.5 | 0.0165 |
| 298.15 | 7.5 | 0.0340 |
| 309.8 | 7.5 | 0.0641 |
| 309.8 | 7.5 | 0.0758 |
| 317.7 | 7.5 | 0.127 |

Reference: 92KRA
Method: HPLC
Buffer: none
pH: 7.5
Evaluation: A

The apparent equilibrium constants given here were obtained from Kragel's Fig. 3.2-1. Kragel also calculated $\Delta_r H'^\circ(\langle T\rangle = 298\ \mathrm{K}, p\mathrm{H} = 7.5) = 17.8\ \mathrm{kJ\ mol^{-1}}$ for this biochemical reaction from the temperature dependency of the apparent equilibrium constant. Also see Kragl *et al.* [91KRA/GYG].

2-oxo-3-deoxy-D-glycero-D-galacto-nonopyranulosonate(aq) =D-mannose(aq)+pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 298.15 | 7.5 | 0.0524 |

Reference: 97SAL/GOD
Method: HPLC
Buffer: none
pH: 7.5
Evaluation: B

N-glycolylneuraminate(aq) = *N*-glycolyl-D-mannosamine(aq)+pyruvate(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 7.2 | 0.090 |

Reference: 62BRU/JOU
Method: radioactivity and spectrophotometry
Buffer: phosphate (0.1 mol dm$^{-3}$)
pH: 7.2
Evaluation: A

### 4.59. Enzyme: chorismate lyase (EC 4.1.3.-)

chorismate(aq)=4-hydroxybenzoate(aq)+pyruvate(aq)

| $T$/K | pH | $I_m$ mol·kg$^{-1}$ | $\Delta_r H$(cal) kJ·mol$^{-1}$ |
|---|---|---|---|
| 298.15 | 6.98 | 0.38 | −144.1 |

Reference: 98TEW/CHE

Method: calorimetry
Buffer: phosphate
pH: 6.98
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -144\ \text{kJ mol}^{-1}$ for the reference reaction: chorismate$^{2-}$(aq)=pyruvate$^{-}$(aq)+4-hydroxybenzoate$^{-}$(aq).

### 4.60. Enzyme: cyclohexa-1,5-diene-1-carboxyl-coenzyme A hydratase (4.2.1.-)

cyclohexa-1,5-diene-1-carboxyl-CoA(aq)+$H_2O(l)$ =6-hydroxycyclohex-1-ene-carboxyl-CoA(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 310.15 | 7.4 | 1.0 |

Reference: 98LAE/EIS
Method: HPLC+radioactivity
Buffer: potassium phosphate (0.1 mol dm$^{-3}$)
pH: 7.4
Evaluation: B

### 4.61. Enzyme: tryptophan synthase (EC 4.2.1.20)

D-glyceraldehyde 3-phosphate(aq)+indole(aq)=1-(indol-3-yl)glycerol 3-phosphate(aq)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 7.5 | −33.8 |

Reference: 85WIE/HIN
Method: calorimetry and spectrophotometry
Buffer: sodium diphosphate (0.1 mol dm$^{-3}$)
pH: 7.5
Evaluation: A

Wiesinger and Hinz reported $\Delta_r H(\text{cal}) = -54.0\ \text{kJ mol}^{-1}$ for this biochemical reaction. However, the reported value included a correction for the hydration of the aldehyde form of D-glyceraldehyde 3-phosphate to its diol form. In the absence of these corrections, the value of $\Delta_r H$(cal) for this reaction is $-33.8\ \text{kJ mol}^{-1}$ (H. Wiesinger, personal communication cited by Kishore *et al.* [98KIS/TEW]). This entry supersedes the entry made in Goldberg and Tewari's [95GOL/TEW] earlier review.

indole(aq)+D-glyceraldehyde 3-phosphate(aq)=1-(indol-3-yl)glycerol 3-phosphate(aq)

| | | $I_m$ | |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | $K'_m$ |
| 298.15 | 7.54 | 0.37 | $1.2\cdot10^4$ |

Reference: 98KIS/TEW
Method: HPLC
Buffer: phosphate
pH: 7.54
Evaluation: A

Kishore *et al.* calculated $K_m(T=298.15\ \text{K}, I=0) = 1.2\cdot10^{-4}$ for the reference reaction: indole$^0$(aq) +D-glyceraldehyde 3-phosphate$^{2-}$(aq)=1-(indol-3-yl)glycerol 3-phosphate$^{2-}$(aq).

indole(aq)+D-glyceraldehyde 3-phosphate(aq)=1-(indol-3-yl)glycerol 3-phosphate(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.26 | 0.37 | −46.9 |

Reference: 98KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 7.26
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -46.9\ \text{kJ mol}^{-1}$ for the reference reaction: indole$^0$(aq)+D-glyceraldehyde 3-phosphate$^{2-}$(aq) =1-(indol-3-yl)glycerol 3-phosphate$^{2-}$(aq).

indole(aq)+L-serine(aq)=L-tryptophan(aq)+$H_2O$(l)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.01 | 0.32 | −74.5 |

Reference: 98KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 7.01
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -74.3\ \text{kJ mol}^{-1}$ for the reference reaction: indole$^0$(aq) +L-serine$^{\pm}$(aq)=L-tryptophan$^{\pm}$(aq)+$H_2O$(l).

1-(indol-3-yl)glycerol 3-phosphate(aq)+L-serine(aq)=L-tryptophan(aq)+D-glyceraldehyde 3-phosphate(aq)+$H_2O$(l)

| | | $\Delta_r H$(cal) |
|---|---|---|
| $T$/K | pH | kJ·mol$^{-1}$ |
| 298.15 | 7.5 | −34 |

Reference: 85WIE/HIN
Method: calorimetry and spectrophotometry
Buffer: sodium diphosphate (0.1 mol dm$^{-3}$)
pH: 7.5
Evaluation: A

Wiesinger and Hinz reported $\Delta_r H(\text{cal}) = -13.4\ \text{kJ mol}^{-1}$ for this biochemical reaction. However, the reported value included a correction for the hydration of the aldehyde form of D-glyceraldehyde 3-phosphate to its diol form. In the absence of these corrections, the value of $\Delta_r H(\text{cal})$ for this reaction is $-34\ \text{kJ mol}^{-1}$ (H. Wiesinger, personal communication cited in Kishore *et al.* [98KIS/TEW]). This entry supersedes the entry made in Goldberg and Tewari's [95GOL/TEW] earlier review.

1-(indol-3-yl)glycerol 3-phosphate(aq) + L-serine(aq) = L-tryptophan(aq) + D-glyceraldehyde 3-phosphate(aq) + $H_2O$(l)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.57 | 0.36 | −27.8 |

Reference: 98KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 7.57
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -27.1\ \text{kJ mol}^{-1}$ for the reference reaction: L-serine$^{\pm}$(aq) + 1-(indol-3-yl)glycerol 3-phosphate$^{2-}$(aq) = L-tryptophan$^{\pm}$(aq) + D-glyceraldehyde 3-phosphate$^{2-}$(aq) + $H_2O$(l).

L-serine(aq) = pyruvate(aq) + ammonia(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 308.15 | 6.90 | 0.39 | −12.1 |

Reference: 98KIS/TEW
Method: calorimetry
Buffer: phosphate
pH: 6.90
Cofactor(s): pyridoxal 5-phosphate and CsCl
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -12.2\ \text{kJ mol}^{-1}$ for the reference reaction: L-serine$^{\pm}$(aq) = pyruvate$^{-}$(aq) + $NH_4^+$(aq).

## 4.62. Enzyme: prephenate dehydratase (EC 4.2.1.51)

prephenate(aq) = phenylpyruvate(aq) + carbon dioxide(aq)

| | | $I_m$ | $\Delta_r H$(cal) |
|---|---|---|---|
| $T$/K | pH | mol·kg$^{-1}$ | kJ·mol$^{-1}$ |
| 298.15 | 7.17 | 0.35 | −127.0 |

Reference: 99KIS/HOL
Method: calorimetry
Buffer: phosphate
pH: 7.17
Evaluation: A

Kishore *et al.* calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -126\ \text{kJ mol}^{-1}$ for the reference reaction: prephenate$^{2-}$(aq) = phenylpyruvate$^{-}$(aq) + $HCO_3^-$(aq).

## 4.63. Enzyme: 4-aminobenzoate synthase (EC 4.-)

chorismate(aq) + ammonia(aq) = 4-amino-4-deoxychorismate(aq) + $H_2O$(l)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 310.15 | 8.6 | 6.1 |

Reference: 91AND/KAT
Method: HPLC
Buffer: Tris (0.050 mol dm$^{-3}$)
pH: 8.6
Cofactor(s): $MgCl_2$ (0.010 mol dm$^{-3}$)
Evaluation: B

This reaction was catalyzed by the PabB subunit of 4-aminobenzoate synthase.

## 4.64. Enzyme: 2-arylpropionyl-coenzyme A epimerase (EC 5.1.2.-)

(*S*)-2-(4-isobutylphenyl)propionyl-CoA(aq) = (*R*)-2-(4-isobutylphenyl)propionyl-CoA(aq)

| $T$/K | pH | $K'_c$ |
|---|---|---|
| 303.15 | 7.0 | 1.5 |

Reference: 93SHI/CHE
Method: HPLC
Buffer: phosphate (0.10 mol dm$^{-3}$)
pH: 7.0
Evaluation: C

## 4.65. Enzyme: UDPglucose 4-epimerase (EC 5.1.3.2)

UDPglucose(aq) = UDPgalactose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.7 | ≈0.33 |

Reference: 60MAX/ROB
Method: spectrophotometry
Buffer: glycine (0.1 mol dm$^{-3}$)
pH: 8.7
Evaluation: C

UDPglucose(aq)=UDPgalactose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.7 | 0.30 |

Reference: 70TSA/HOL
Method: spectrophotometry
Buffer: glycine (0.1 mol dm$^{-3}$)+NaOH
pH: 8.7
Evaluation: A

UDPglucose(aq)=UDPgalactose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.7 | 0.29 |

Reference: 80FUK/OBO
Method: spectrophotometry
Buffer: glycine (0.1 mol dm$^{-3}$)+NaOH
pH: 8.7
Evaluation: B

UDPglucose(aq)=UDPgalactose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.5 | 0.29 |

Reference: 96PRO/GRO
Method: spectrophotometry
Buffer: Tris (0.020 mol dm$^{-3}$)+HCl
pH: 8.5
Cofactor(s): $MgCl_2$ (0.001 mol dm$^{-3}$)
Evaluation: C

### 4.66. Enzyme: *N*-acylglucosamine 2-epimerase (EC 5.1.3.8)

*N*-acetyl-D-glucosamine(aq)=*N*-acetyl-D-mannosamine(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.5 | 0.201 |

Reference: 92KRA
Method: HPLC
Buffer: none
pH: 7.5
Evaluation: A

### 4.67. Enzyme: xylose isomerase (EC 5.3.1.5)

D-glucose(aq)=D-fructose(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 333.15 | 7.0 | 0.98 |
| 338.15 | 7.0 | 1.03 |
| 343.15 | 7.0 | 1.14 |
| 348.15 | 7.0 | 1.22 |
| 353.15 | 7.0 | 1.39 |

Reference: 97CON/DEL
Method: HPLC
Buffer: Tris (0.05 mol dm$^{-3}$)
pH: 7.0
Cofactor(s): $MgSO_4$
Evaluation: C

We calculate $\Delta_r H'°(\langle T\rangle = 343.15$ K, pH=7.0)=16.9 kJ mol$^{-1}$ from the temperature dependency of the apparent equilibrium constant.

### 4.68. Enzyme: glucose-6-phosphate isomerase (EC 5.3.1.9)

D-glucose 6-phosphate(aq)=D-fructose 6-phosphate(aq)

| $T$/K | pH | buffer | $K'$ |
|---|---|---|---|
| 310.15 | 7.0 | Imidazole | 0.33 |
| 310.15 | 8.0 | Tris | 0.30 |

Reference: 97STA/SUA
Method: spectrophotometry
Buffer: Imidazole (0.025 mol dm$^{-3}$) and Tris (0.025 mol dm$^{-3}$)
pH: 7.0–8.0
Cofactor(s): $MgCl_2$ (0.005 mol dm$^{-3}$)
Evaluation: A

### 4.69. Enzyme: phosphoglucomutase (EC 5.4.2.2)

α-D-glucose 1-phosphate(aq)=α-D-glucose 6-phosphate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 3.7 |

Reference: 96OES/SCH
Method: enzymatic assay and spectrophotometry
Buffer: Tris (0.050 mol dm$^{-3}$)+HCl
pH: 7.0
Cofactor(s): $MgCl_2$ (0.001 mol dm$^{-3}$)
Evaluation: B

Also see data given under phosphomannomutase (EC 5.4.2.8) [95GOL/TEW].

### 4.70. Enzyme: phosphomannomutase (EC 5.4.2.8)

α-D-glucose 1-phosphate(aq)=α-D-glucose 6-phosphate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 1.4 |

Reference: 96OES/SCH
Method: enzymatic assay and spectrophotometry
Buffer: Tris (0.050 mol dm$^{-3}$)+HCl
pH: 7.0
Cofactor(s): $MgCl_2$ (0.001 mol dm$^{-3}$)
Evaluation: B

Also see data given under β-phosphoglucomutase (EC 5.4.2.6) [95GOL/TEW].

D-mannose 1-phosphate(aq) = D-mannose 6-phosphate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.0 | 1.0 |

Reference: 96OES/SCH
Method: enzymatic assay and spectrophotometry
Buffer: Tris (0.050 mol $dm^{-3}$)+HCl
pH: 7.0
Cofactor(s): $MgCl_2$ (0.001 mol $dm^{-3}$)
Evaluation: B

### 4.71. Enzyme: chorismate mutase (EC 5.4.99.5)

chorismate(aq)=prephenate(aq)

| $T$/K | pH | buffer | $I_m$ / mol·$kg^{-1}$ | $\Delta_r H$(cal) / kJ·$mol^{-1}$ |
|---|---|---|---|---|
| 298.15 | 6.93 | phosphate | 0.18 | −55.5 |
| 298.15 | 7.70 | Tris | 0.071 | −55.4 |

Reference: 97KAS/TEW
Method: calorimetry
Buffer: phosphate and Tris
pH: 6.93
Evaluation: A

Kast *et al.* also calculated $\Delta_r H°(T=298.15\ \text{K}, I=0) = -55.4\ \text{kJ mol}^{-1}$ for the reference reaction: $\text{chorismate}^{2-}(\text{aq}) = \text{prephenate}^{2-}(\text{aq})$. This study was complemented by a quantum mechanical calculation of $\Delta_r H°$ for this reference reaction.

### 4.72. Enzyme: isochorismate synthase (EC 5.4.99.6)

chorismate(aq)=isochorismate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 7.5 | 0.66 |

Reference: 90LIU/QUI
Method: NMR and spectrophotometry
Buffer: phosphate (0.050 mol $dm^{-3}$)
pH: 7.5
Cofactor(s): $MgCl_2$ (0.005 mol $dm^{-3}$)
Evaluation: A

The value $K' = 0.56$ was also obtained from kinetic data and by using the Haldane relationship. The same results are also given in Liu's thesis [90LIU].

chorismate(aq)=isochorismate(aq)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.0 | 0.55 |

Reference: 95KOZ/TOM
Method: HPLC
Buffer: $(NH_4)_2SO_4$ (0.050 mol $dm^{-3}$)
pH: 8.0
Evaluation: C

The temperature was assumed to be 298.15 K.

chorismate(aq) + ammonia(aq) = 2-amino-2-deoxyisochorismate(aq)+$H_2O$(l)

| $T$/K | pH | $K'$ |
|---|---|---|
| 298.15 | 8.0 | 2.67 |

Reference: 95KOZ/TOM
Method: HPLC
Buffer: $(NH_4)_2SO_4$ (0.050 mol $dm^{-3}$)
pH: 8.0
Evaluation: C

The temperature was assumed to be 298.15 K.

## 5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers

| Substance | CAS Registry Number[a] | Enzyme Commission Numbers |
|---|---|---|
| acetaldehyde | 75-07-0 | 1.1.1.1 |
| acetate | 64-19-7 | 3.5.1.14 |
| acetyl-coenzyme A | 72-89-9 | 2.31.30 |
| *N*-acetyl-D-glucosamine | 7512-17-6 | 5.1.3.8 |
| *N*-acetyl-D-mannosamine | 3615-17-6 | 4.1.3.3, 5.1.3.8 |
| *N*-acetyl-L-methionine | 65-82-7 | 3.5.1.14 |
| *N*-acetylneuraminate | 131-48-6 | 4.1.3.3 |
| *N*-acetyl-L-phenylalanine | 2018-61-3 | 3.4.21.1 |
| *N*-acetyl-L-phenylalanine ethyl ester | 2361-96-8 | 3.4.21.1 |
| *O*-acetyl-L-serine | 66638-22-0 | 2.3.1.30 |
| *N*-acetyl-L-tryptophan | 1218-34-4 | 3.4.21.1 |
| *N*-acetyl-L-tryptophan ethyl ester | 2382-80-1 | 3.4.21.1 |
| *N*-acetyl-L-tyrosine | 537-55-3 | 3.4.21.1 |
| *N*-acetyl-L-tyrosine ethyl ester | 36546-50-6 | 3.4.21.1 |
| adenosine 5′-diphosphate | 58-64-0 | 2.7.1.32, 2.7.2.3, 2.7.3.3, 2.7.3.4, 2.7.4.3, 2.7.4.8 |
| adenosine 5′-monophosphate | 61-19-8 | 2.7.4.3 |
| adenosine 5′-triphosphate | 56-65-5 | 2.7.1.32, 2.7.2.3, 2.7.3.3, 2.7.3.4, 2.7.4.3, 2.7.4.8, 2.7.7.42 |
| adenylyl-[L-glutamate:ammonia ligase (ADP-forming)] | 155039-15-9 | 2.7.7.42 |
| L-alanine | 56-41-7 | 2.6.1.-, 2.6.1.2 |
| allantoin | 97-59-6 | 1.7.3.3, 1.11.1.6 |
| *allo*lactose | 28447-39-4 | 3.2.1.23 |
| 7-aminodeacetoxycephalosporanic acid | 22252-43-3 | 3.5.1.- |
| 4-amino-4-deoxychorismate | 97279-79-3 | 4.- |
| 2-amino-2-deoxyisochorismate | 214403-80-2 | 5.4.99.6 |
| (*S*)-aminomethyldihydro-$\alpha$-lipoate | 214403-81-3 | 1.4.4.2 |
| 6-aminopenicillanic acid | 551-16-6 | 3.5.1.11, 3.5.1.- |
| D(-)-$\alpha$-aminophenylacetic acid | 875-74-1 | 3.5.1.- |
| 3-aminopropionaldehyde | 352-92-1 | 2.6.1.- |
| ammonia | 7664-41-7 | 3.5.1.1, 3.5.1.2, 3.5.1.5, 4.2.1.20, 4.-, 5.4.99.6 |
| ammonium carbamate | 1111-78-0 | 3.5.1.5 |
| amoxicillin | 61336-70-7 | 3.5.1.11 |
| ampicillin | 69-53-4 | 3.5.1.- |
| D-arabitol | 488-82-4 | 1.1.1.14 |
| L-arginine | 74-79-3 | 2.7.3.3, 3.5.3.1 |
| L-asparagine | 70-47-3 | 3.5.1.1 |
| L-aspartate | 56-84-8 | 2.6.1.1, 3.5.1.1 |
| *N*-(benzyloxycarbonyl-L-aspartic acid | 1152-61-0 | 3.4.24.27 |
| *N*-(benzyloxycarbonyl)-L-aspartyl-L-phenylalanine methyl ester | 33605-72-0 | 3.4.24.27 |
| (*Z*)=*enol*butyryl-UDP-*N*-acetylglucosamine | 56374-30-2 | 2.5.1.7 |
| (+)-camphor | 464-49-3 | 1.14.15.1 |
| carbon dioxide | 124-38-9 | 1.3.1.12, 1.4.4.2, 1.7.3.3, 1.11.1.6, 3.5.1.5, 4.2.1.51 |
| D-carnitine | 541-14-0 | 1.1.1.108 |
| cellobiose | 528-50-7 | 2.4.1.20 |

5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers—Continued

| Substance | CAS Registry Number[a] | Enzyme Commission Numbers |
|---|---|---|
| cephalexin | 15686-71-2 | 3.51.- |
| cholest-4-en-3-one | 601-57-0 | 1.1.3.6, 1.11.1.6 |
| cholesterol | 57-88-5 | 1.1.3.6, 1.11.1.6, 4.1.3.-, 4.-, 5.4.99.5, 5.4.99.6 |
| choline | 62-49-7 | 2.7.1.32 |
| chorismate | 55508-12-8 | 4.1.3.-, 4.-, 5.4.99.5, 5.4.99.6 |
| coenzyme A | 85-61-0 | 2.3.1.30 |
| creatine | 57-00-1 | 2.7.3.2 |
| cyclocreatine | 35404-50-3 | 2.7.3.2 |
| cyclohexa-1,5-diene-1-carboxyl-coenzyme A | 148471-94-7 | 4.2.1.- |
| cyclomaltoheptaose | 7585-39-9 | 2.4.1.19, 3.2.1.1, 3.2.1.3 |
| cyclomaltohexaose | 10016-20-3 | 2.4.1.19, 3.2.1.3 |
| cyclomaltooctaose | 17465-86-0 | 2.4.1.19, 3.2.1.1, 3.2.1.3 |
| (*R*)-2-decanol | 33758-15-5 | 3.1.1.3 |
| (*R*)-2-decyl butyrate | 128942-08-5 | 3.1.1.3 |
| 3-dehydrocarnitine | 10457-99-5 | 1.1.1.108 |
| 1,3-diaminopropane | 109-76-2 | 2.6.1.- |
| dihydro-$\alpha$-lipoate | 462-20-4 | 1.8.1.4 |
| (*S*)-dihydroorotate | 5988-19-2 | 1.3.99.11 |
| dihydroxonic acid | 499-09-2 | 1.3.99.11 |
| dodecanal | 112-54-9 | 1.14.14.3 |
| 1-dodecanoic acid | 143-07-7 | 1.14.14.3, 3.1.1.3 |
| 1-dodecanol | 112-53-8 | 3.1.1.3 |
| (*R*)-2-dodecanol | 99210-87-4 | 3.1.1.3 |
| (*R*)-2-dodecyl butyrate | 99113-82-3 | 3.1.1.3 |
| dodecyl dodecanoate | 13945-76-1 | 3.1.1.3 |
| ethanol | 64-17-5 | 3.4.21.1, 1.1.1.1 |
| ethyl-(*E*)-2-octenoate | 2351-90-8 | 2.5.1.18 |
| D-fructose | 57-48-7 | 1.1.1.14, 1.1.1.67, 2.4.1.13, 3.2.1.3, 3.2.1.23, 3.2.1.26, 5.3.1.5 |
| D-fructose 6-phosphate | 643-13-0 | 5.3.1.9 |
| 6-*O*-$\alpha$-D-galactopyranosyl-D-galactopyranose | 13117-25-4 | 3.2.1.3 |
| D-galactose | 59-23-4 | 3.2.1.3, 3.2.1.23 |
| D-glucono-1,5-lactone | 90-80-2 | 1.1.3.4, 1.11.1.6 |
| 4-*O*-$\alpha$-D-glucopyranosyl-D-fructofuranose | 17606-72-3 | 3.2.1.3 |
| 3-*O*-$\alpha$-D-glucopyranosyl-lyxopyranose | 197901-78-3 | 3.2.1.3 |
| D-glucose | 50-99-7 | 2.4.1.19, 2.4.1.20, 3.2.1.1, 3.2.1.3, 3.2.1.23, 3.2.1.26, 5.3.1.5 |
| $\beta$-D-glucose | 492-61-5 | 1.1.3.4, 1.11.1.6 |
| $\alpha$-D-glucose 1-phosphate | 59-56-3 | 2.4.1.20, 2.7.7.9, 2.7.7.-, 5.4.2.2, 5.4.2.8 |
| D-glucose 6-phosphate | 56-73-5 | 5.3.1.9 |
| $\alpha$-D-glucose 6-phosphate | 15209-11-7 | 5.4.2.2, 5.4.2.8 |
| L-glutamate | 56-86-0 | 2.6.1.1, 2.6.1.2, 2.6.1.5, 2.6.1.42, 3.5.1.2 |
| L-glutamate:ammonia ligase (ADP-forming) | 9023-70-5 | 2.7.7.42 |
| L-glutamine | 56-85-9 | 3.5.1.2 |
| glutathione (oxidized) | 103239-24-3 | 1.6.4.2 |
| glutathione (reduced) | 70-18-8 | 1.6.4.2, 2.5.1.18. |

5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers—Continued

| Substance | CAS Registry Number[a] | Enzyme Commission Numbers |
|---|---|---|
| glutathionyl-ethyl-(*E*)-2-octenoate | 214403-82-4 | 2.5.1.18 |
| glutathionyl-methyl-(*E*)-2-octenoate | 214403-83-5 | 2.5.1.18 |
| glutathionyl-(*E*)-3-nonen-2-one | 214403-84-6 | 2.5.1.18 |
| glutathionyl-(*E*)-2-octenal | 214403-85-7 | 2.5.1.18 |
| 4-(glutathionyl)-4-phenyl-2-butanone | 104786-88-1 | 2.5.1.18 |
| D-glyceraldehyde 3-phosphate | 142-10-9 | 4.2.1.20 |
| glycerol-1,2-dibutyrate | 24814-35-5 | 3.1.1.3 |
| glycine | 56-40-6 | 1.4.4.2, 2.1.2.1 |
| *N*-glycolyl-D-mannosamine | 7483-19-4 | 4.1.3.3 |
| *N*-glycolylneuraminate | 113-83-3 | 4.1.3.3 |
| *β*-guanidinopropionate | 353-09-3 | 2.7.3.2 |
| guanosine 2′:3′-(cyclic)phosphate | 15718-49-7 | 3.1.27.5 |
| guanosine 5′-diphosphate | 146-91-8 | 2.7.4.8 |
| guanosine 3′-methylphosphate | 69414-27-3 | 3.1.27.5 |
| guanosine 3′-monophosphate | 6027-83-4 | 3.1.27.5 |
| guanosine 5′-monophosphate | 85-32-5 | 2.7.4.8 |
| $H_2O$ | 7732-18-5 | 1.1.3.4, 1.1.3.6, 1.3.1.12, 1.7.3.3, 1.11.1.6, 1.11.1.7, 1.14.14.3, 1.14.15.1, 2.1.2.1, 2.4.1.19, 3.1.1.3, 3.1.1.20, 3.1.27.5, 3.2.1.1, 3.2.1.3, 3.2.1.23, 3.2.1.26, 3.4.21.1, 3.4.24.27, 3.5.1.1, 3.5.1.2, 3.5.1.5, 3.5.1.14, 3.5.1.-, 3.5.3.1, 4.2.1.20, 4.2.1.-, 4.-, 5.4.99.6 |
| $H_2O_2$ | 7722-84-1 | 1.1.3.4, 1.1.3.6, 1.11.1.6, 1.11.1.7 |
| (*R*)-2-heptanol | 6033-24-5 | 3.1.1.3 |
| (*R*)-2-heptyl butyrate | 117636-45-0 | 3.1.1.3 |
| hippurate | 495-69-2 | 3.4.21.1 |
| 4-hydroxybenzoate | 99-96-7 | 4.1.3.- |
| (+)-5-*exo*-hydroxycamphor | 1607-84-7 | 1.14.15.1 |
| 6-hydroxycyclohex-1-ene-carboxyl-coenzyme A | 148471-95-8 | 4.2.1.- |
| D-4-hydroxyphenylglycine | 22818-40-2 | 3.5.1.11 |
| 4-hydroxyphenylpyruvate | 156-39-8 | 1.3.1.12, 2.6.1.5 |
| L-iditol | 488-45-9 | 1.1.1.14 |
| imidazole | 288-32-4 | 2.7.7.- |
| indole | 120-72-9 | 4.2.1.20 |
| 1-(indol-3-yl)glycerol 3-phosphate | 4220-97-7 | 4.2.1.20 |
| (*R*)-2-(4-isobutylphenyl)propionyl-coenzyme A | 105567-78-0 | 5.1.2.- |
| (*S*)-2-(4-isobutylphenyl)propionyl-coenzyme A | 135027-64-4 | 5.1.2.- |
| isochorismate | 22642-82-6 | 5.4.99.6 |
| *α*-isomaltose | 499-40-1 | 3.2.1.3 |
| *β*-isomaltose | 22352-61-0 | 3.2.1.3 |
| (*S*)-lactate | 79-33-4 | 1.1.1.27 |
| lactose | 63-42-3 | 3.2.1.23 |
| lactulose | 4618-18-2 | 3.2.1.23 |
| L-leucine | 61-90-5 | 2.6.1.42 |
| *α*-lipoate | 1077-28-7 | 1.4.4.2, 1.8.1.4 |
| lyxose | 1114-34-7 | 3.2.1.3 |
| D-mannitol | 69-65-8 | 1.1.1.14, 1.1.1.67 |

5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers—Continued

| Substance | CAS Registry Number[a] | Enzyme Commission Numbers |
|---|---|---|
| 1-*O*-α-D-mannopyranosyl-D-mannofuranose | 197902-09-3 | 3.2.1.3 |
| 6-*O*-α-D-mannopyranose-D-mannopyranose | 6614-35-3 | 3.2.1.3 |
| D-mannose | 3458-28-4 | 3.2.1.3, 4.1.3.3 |
| D-mannose 1-phosphate | 51306-17-3 | 5.4.2.8 |
| D-mannose-6-phosphate | 70442-25-0 | 5.4.2.8 |
| α-D-melibiose | 585-99-9 | 3.2.1.3 |
| β-D-melibiose | 29873-67-4 | 3.2.1.3 |
| (−)-menthol | 2216-51-5 | 3.1.1.3 |
| (−)-menthyl dodecanoate | 57084-14-7 | 3.1.1.3 |
| methanol | 67-56-1 | 3.1.27.5 |
| L-methionine | 63-68-3 | 3.5.1.14 |
| 5,10-methylenetetrahydrofolate | 3432-99-3 | 2.1.2.1 |
| methyl-(*E*)-octenoate | 2396-85-2 | 2.5.1.18 |
| 4-methyl-2-oxopentanooate | 816-66-0 | 2.6.1.42 |
| β-nicotinamide-adenine dinucleotide (oxidized) | 53-84-9 | 1.1.1.1, 1.1.1.27, 1.1.1.56, 1.1.1.108, 1.1.1.141, 1.3.1.12, 1.6.4.2, 1.8.1.4, 1.14.15.1 |
| β-nicotinamide-adenine dinucleotide (reduced) | 606-68-8 | 1.1.1.1, 1.1.1.27, 1.1.1.56, 1.1.1.108, 1.1.1.141, 1.3.1.12, 1.6.4.2, 1.8.1.4, 1.14.15.1 |
| β-nicotinamide-adenine dinucleotide phosphate (oxidized) | 53-59-8 | 1.1.1.67, 1.6.4.2 |
| β-nicotinamide-adenine dinucleotide phosphate (reduced) | 2646-71-1 | 1.1.1.67, 1.6.4.2 |
| (*R*)-2-nonanol | 628-99-9 | 3.1.1.3 |
| (*E*)-3-none-2-one | 14309-57-0 | 2.5.1.18 |
| (*R*)-2-nonyl butyrate | 117636-46-1 | 3.1.1.3 |
| $O_2$ | 7782-44-7 | 1.1.3.4, 1.1.3.6, 1.7.3.3, 1.11.1.6, 1.14.14.1, 1.14.15.3 |
| (*E*)-2-octenal | 2548-87-0 | 2.5.1.18 |
| (*R*)-2-octanol | 5978-70-1 | 3.1.1.3 |
| (*R*)-2-octyl butyrate | 89378-60-9 | 3.1.1.3 |
| L-ornithine | 70-26-8 | 3.5.3.1 |
| orotate | 65-86-1 | 1.3.99.11 |
| orthophosphate | 10049-21-5 | 2.4.1.20, 2.5.1.7 |
| oxaloacetate | 328-42-7 | 2.6.1.1 |
| 2-oxo-3-deoxy-D-glycero-D-galacto-nonopyranulosonate | 124233-95-0 | 4.1.3.3 |
| 2-oxoglutarate | 328-50-7 | 2.6.1.1, 2.6.1.2, 2.6.1.5, 2.6.1.42 |
| oxonic acid | 2207-75-2 | 1.3.99.11 |
| 15-oxo-prostaglandin $E_2$ | 26441-05-4 | 1.1.1.141 |
| L-phenylalanine | 63-91-2 | 2.6.1.5 |
| L-phenylalanine methyl ester | 2577-90-4 | 3.4.24.27 |
| (*E*)-4-phenyl-3-buten-2-one | 1896-62-4 | 2.5.1.18 |
| phenylpyruvate | 156-06-9 | 2.6.1.5, 4.2.1.51 |
| $N^{\omega}$-phospho-L-arginine | 108321-86-4 | 2.7.3.3 |
| (*Z*)-phospho*enol*butyrate | 31302-64-4 | 2.5.1.7 |
| *O*-phosphocholine | 107-73-3 | 2.7.1.32 |
| phosphocreatine | 6190-45-0 | 2.7.3.2 |
| phosphocyclocreatine | 61839-19-8 | 2.7.3.2 |
| 3-phospho-D-glycerate | 820-11-1 | 2.7.2.3 |

5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers—Continued

| Substance | CAS Registry Number[a] | Enzyme Commission Numbers |
|---|---|---|
| 3-phospho-D-glyceroyl phosphate | 38168-82-0 | 2.7.2.3 |
| $\beta$-phosphoguanidinopropionate | 55601-59-7 | 2.7.3.2 |
| $N^{\omega}$-phosphotaurocyamine | 4189-99-5 | 2.7.3.4 |
| prephenate | 126-49-8 | 1.3.1.12, 4.2.1.51, 5.4.99.5 |
| 1-propanol | 71-23-8 | 3.1.1.20 |
| 2-propanol | 67-63-0 | 3.4.21.1 |
| 2-propylhippurate | 1776-56-3 | 3.4.21.1 |
| prostaglandin $E_2$ | 363-24-6 | 1.1.141 |
| pyrophosphate | 2466-09-3 | 2.7.7.9, 2.7.7.42 |
| pyruvate | 127-17-3 | 1.1.1.27, 2.6.1.2, 2.6.1.-, 4.1.3.3, 4.1.3.-, 4.2.1.20 |
| ribitol | 488-81-3 | 1.1.1.56 |
| riboflavin 5′-phosphate (oxidized) | 146-17-8 | 1.14.14.3 |
| riboflavin 5′-phosphate (reduced) | 5666-16-0 | 1.14.14.3 |
| D-ribulose | 488-84-6 | 1.1.1.14, 1.1.1.56 |
| L-serine | 56-45-1 | 2.1.2.1, 2.3.1.30, 4.2.1.20 |
| D-sorbitol | 50-70-4 | 1.1.1.14 |
| L-sorbose | 87-79-6 | 1.1.1.14 |
| sucrose | 57-50-1 | 2.4.1.13, 3.2.1.26 |
| taurocyamine | 543-18-0 | 2.7.3.4 |
| tetraglutamyl-5,10-methylenetetrahydrofolate | 60283-91-2 | 2.1.2.1 |
| tetraglutamyl-5,6,7,8-tetrahydrofolate | 50998-24-8 | 2.1.2.1 |
| 5,6,7,8-tetrahydrofolate | 135-16-0 | 2.1.2.1 |
| thiocyanate (oxidized) | 63296-34-4 | 1.11.1.7 |
| thiocyanate (reduced) | 463-56-9 | 1.11.1.7 |
| tributyrylglycerol | 60-01-5 | 3.1.1.3 |
| 3,4,5-trihydroxybenzoate | 149-91-7 | 3.1.1.20 |
| 3,4,5-trihydroxybenzoic acid propyl ester | 121-79-9 | 3.1.1.20 |
| L-trytophan | 73-22-3 | 4.2.1.20 |
| L-tyrosine | 60-18-4 | 2.6.1.5 |
| (*R*)-2-undecanol | 85617-06-7 | 3.1.1.3 |
| (*R*)-2-undecyl butyrate | 181148-07-2 | 3.1.1.3 |
| urate | 69-93-2 | 1.7.3.3, 1.11.1.6 |
| urea | 57-13-6 | 3.5.1.5, 3.5.3.1 |
| uridine 2′:3′-(cyclic)phosphate | 15718-50-0 | 3.1.27.5 |
| uridine 5′-diphosphate | 58-98-0 | 2.4.1.13 |
| uridine 5′-diphospho-*N*-acetyl-D-glucosamine | 91183-98-1 | 2.5.1.7 |
| uridine 5′-diphosphogalactose | 89705-69-1 | 5.1.3.2 |
| uridine 5′-diphosphoglucose | 133-89-1 | 2.4.1.13, 2.7.7.9, 2.7.7.-, 5.1.3.2 |
| uridine 5′-phosphoimidazole | 214403-86-8 | 2.7.7.- |
| uridine 3′-monophosphate | 35170-03-7 | 3.1.27.5 |
| uridine 5′-triphosphate | 63-39-8 | 2.7.7.9 |
| xylitol | 87-99-0 | 1.1.1.14 |
| D-xylulose | 551-84-8 | 1.1.1.14 |

[a]In some cases the CAS registry number refers to a salt of the substance.

## 6. Abbreviations

| | | | |
|---|---|---|---|
| ADP | adenosine 5′-diphosphate | Mops | 3-morpholinopropanesulfonic acid |
| AMP | adenosine 5′-monophosphate | NAD | β-nicotinamide-adenine dinucleotide (oxidized) |
| ATP | adenosine 5′-triphosphate | NADH | β-nicotinamide-adenine dinucleotide (reduced) |
| Bicine | *N*,*N*-bis(2-hydroxyethyl)glycine | NADP | β-nicotinamide-adenine dinucleotide phosphate (oxidized) |
| Ches | 2-(cyclohexylamino)ethanesulfonic acid | NADPH | β-nicotinamide-adenine dinucleotide phosphate (reduced) |
| CoA | coenzyme A | Pipes | piperazine-*N*,*N*′-bis(2-ethanesulfonic acid) |
| GDP | guanosine 5′-diphosphate | Tes | *N*-tris(hydroxymethyl)methyl-2-aminoethane-sulfonic acid |
| Hepes | *N*-(2-hydroxyethyl)piperazine-*N*′-ethanesulfonic acid | Tris | tris(hydroxymethyl)aminomethane |
| Mes | 2-(*N*-morpholino)ethanesulfonic acid | UDP | uridine 5′-diphosphate |

## 7. Glossary of Symbols

| Symbol | Name | Unit |
|---|---|---|
| $c$ | concentration | $\mathrm{mol\,dm^{-3}}$ |
| $c^\circ$ | standard concentration ($c^\circ = 1\,\mathrm{mol\,dm^{-3}}$) | $\mathrm{mol\,dm^{-3}}$ |
| $\Delta_r C_p^\circ$ | standard heat capacity of reaction at constant pressure | $\mathrm{J\,K^{-1}\,mol^{-1}}$ |
| $\Delta_r G^\circ$ | standard Gibbs energy of reaction | $\mathrm{kJ\,mol^{-1}}$ |
| $\Delta_r G'^\circ$ | standard transformed Gibbs energy of reaction | $\mathrm{kJ\,mol^{-1}}$ |
| $\Delta_r H^\circ$ | standard enthalpy of reaction | $\mathrm{kJ\,mol^{-1}}$ |
| $\Delta_r H'^\circ$ | standard transformed enthalpy of reaction | $\mathrm{kJ\,mol^{-1}}$ |
| $\Delta_r H(\mathrm{cal})$ | calorimetrically determined enthalpy of reaction | $\mathrm{kJ\,mol^{-1}}$ |
| $I_c$ | ionic strength, concentration basis | $\mathrm{mol\,dm^{-3}}$ |
| $I_m$ | ionic strength, molality basis | $\mathrm{mol\,kg^{-1}}$ |
| $K$ | equilibrium constant[a] | dimensionless |
| $K'$ | apparent equilibrium constant[a] | dimensionless |
| $m$ | molality | $\mathrm{mol\,kg^{-1}}$ |
| $m^\circ$ | standard molality ($m^\circ = 1\,\mathrm{mol\,kg^{-1}}$) | $\mathrm{mol\,kg^{-1}}$ |
| $\Delta_r N(\mathrm{H^+})$ | change in binding of hydrogen ion in a biochemical reaction | dimensionless |
| $P$ | pressure | Pa |
| pH | $-\log_{10}\{c(\mathrm{H^+})/c^\circ\}$[b] | dimensionless |
| pX | $-\log_{10}\{c(X)/c^\circ\}$ | dimensionless |
| $\Delta_r S^\circ$ | standard entropy of reaction | $\mathrm{J\,K^{-1}\,mol^{-1}}$ |
| $T$ | thermodynamic temperature | K |
| $x$ | mole fraction | dimensionless |

[a]When needed, a subscript $c$, $m$, or $x$ is added to these quantities to designate a concentration, molality, or mole fraction basis.

[b]This is an approximate definition. The IUPAC Green Book [I. Mills, T. Cvitaš, K. Homann, N. Kallay, and K. Kuchitsu, *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific, Oxford, 1993)] contains a discussion of the operational definition of pH.

## 8. Reference Codes and References in the Table


50PAZ Pazur, J. H., "Mathematical Analysis of Amylase Action," thesis, Iowa State College (1950).

58BAC Backlin, K.-I., Acta Chem. Scand. **12**, 1279 (1958).

59SAN/LAN Sanadi, D. R., Langley, M., Searls, R. L., J. Biol. Chem. **234**, 178 (1959).

60MAX/ROB Maxwell, E. S., deRobichoin-Szulmajster, H., J. Biol. Chem. **235**, 308 (1960).

61ALE Alexander, J. K., J. Bacteriol. **81**, 903 (1961).

62BRU/JOU Brunetti, P., Jourdian, G. W., Roseman, S., J. Biol. Chem. **237**, 2447 (1962).

62COM/ROS Comb, D. G., Roseman, S., Methods Enzymol. **5**, 391 (1962).

64ROS/RAP Rost, J., Rapoport, S., Nature **201**, 185 (1964).

68BRO Brosnan, J. T., "Studies Related to Ammonia Metabolism in Animal Tissues," thesis, Oxford University (1968).

69PET/MCK Peterson, J. A., McKenna, E. J., Estabrook, R. W., Coon, M. J., Arch. Biochem. Biophys. **131**, 245 (1969).

69ROS/HAM del Rosario, E. J., Hammes, G. G., Biochemistry **8**, 1884 (1969).

69TSU Tsuboi, K. K., Fukunaga, K., Petricciani, J. C., J. Biol. Chem. **244**, 1008 (1969).

70BRO/KRE Brosnan, J. T., Krebs, H. A., Williamson, D. H., Biochem. J. **117**, 91 (1970).

70JEN/TAY Jenkins, W. T., Taylor, W. T., Methods Enzymol. **17A**, 802 (1970).

70TSA/HOL Tsai, C. M., Holmberg, N., Ebner, K. E., Arch. Biochem. Biophys. **136**, 233 (1970).

71RAJ/LUM Rajender, S., Lumry, R., Han, M. J. Phys. Chem. **75**, 1375 (1971).

71WOH Wohlhueter, R. M., Eur. J. Biochem. **21**, 575 (1971).

72NEL/KIE Nelson, D. P., Kiesow, L. A., Anal. Biochem. **49**, 474 (1972).

74BUR Burton, K., Biochem. J. **143**, 365 (1974).

75GOR/ESF Gorin, G., Esfandi, A., Guthrie, G. B., Jr., Arch. Biochem. Biophys. **168**, 450 (1975).

75MAN/LAN Mangold, A., Langerman, N., Arch. Biochem. Biophys. **169**, 126 (1975).

75SCH/GRE Schlegel, W., Greep, R. O., Eur. J. Biochem. **56**, 245 (1975).

76SCH/KRI Schmidt, H.-L., Krisam, G., Grenner, G., Biochim. Biophys. Acta **429**, 283 (1976).

77REH/JAN Rehak, N. N., Janes, G., Young, D. S., Clin. Chem. (Winston-Salem, N. C.) **23**, 195 (1977).

77SCH/TAT Schirch, L. V., Tatum, C. M., Jr., Benkovic, S. J., Biochemistry **16**, 410 (1977).

78MCG/BRO McGuinness, E. T., Brown, H. D., Chattopadhyay, S. K., Chen, F., Biochim. Biophys. Acta **530**, 247 (1978).

80FUK/OBO Fukasawa, T., Obonai, K., Segawa, T., Nogi, Y., J. Biol. Chem. **255**, 2705 (1980).

82REH/YOU Rehak, N. N., Young, D. S., Clin. Chem. (Winston-Salem, N. C.) **28**, 2235 (1982).

84OYA/IRI Oyama, K., Irino, S., Harada, T., Hagi, N., in *Enzyme Engineering* 7, A. I. Laskin, G. T. Tsao, and L. B. Wingard, eds.; New York Academy of Sciences, New York (1984). pp. 95–98.

84UCH/TSU Uchida, Y., Tsukada, Y., Sugimori, T., J. Biochem. (Tokyo) **96**, 507 (1984).

85LIE Liegel, J., "The Equilibrium Constant for the Glycine Synthase Reaction," thesis, The University of Texas (1985).

85WIE/HIN Wiesinger, H., Hinz, H. J., Arch. Biochem. Biophys. **242**, 440 (1985).

86MEY/BRO Meyer, R. A., Brown, T. R., Krilowicz, B. L. Kushmerick, M. J., Am. J. Physiol. **250**, C264 (1986)

86NAK/KIM Nakanishi, K., Kimura, Y., Matsuno, R., Eur. J Biochem. **161**, 541 (1986).

86PRU/TEN Pruitt, K. M., Tenovuo, J., Mansson-Rahemtulla, B. Harrington, P., Baldone, D. C., Biochim. Biophys Acta **870**, 385 (1986).

89JEE/SHI Jee, J.-G., Shin, J.-Y., Bull Korean Chem. Soc. **10**, 5( (1989).

89SCH/GIF Schneider, K.-H., Giffhorn, F., Eur. J. Biochem. **184** 15 (1989).

90LIU Liu, J., "Molecular Studies on Enzymes in the Enterobactin Biosynthetic Pathway and on Peptidyl-Prolyl Cis-Trans Isomerase," thesis, Massachusetts Institute of Technology (1990).

90LIU/QUI Liu, J., Quinn, N., Berchtold, G. A., Walsh, C. T., Biochemistry **29**, 1417 (1990).

91AND/KAT Anderson, K. S., Kati, W. M., Ye, Q.-Z., Liu, J., Walsh, C. T., Benesi, A. J., Johnson, K. A., J. Am. Chem. Soc. **113**, 3198 (1991).

91HOR/UEH Hori, N., Uehara, K., Mikami, Y., Agric. Biol. Chem. **55**, 1071 (1991).

91KRA/GYG Kragl, U., Gygax, D., Ghisalba, O., Wandrey, C., Angew. Chem. **103**, 854 (1991); Angew. Chem. Int. Ed. Engl. **30**, 827 (1991).

92ELL/SRI Elliott, A. C., Srinivasan, K., Sinnott, M. L., Smith, P. J., Bommuswamy, J., Guo, Z., Hall, B. G., Zhang, Y., Biochem. J. **282**, 155 (1992).

92KAH/SCH Kahle, C., Schneider, K.-H., Giffhorn, F., J. Gen. Microbiol. **138**, 1277 (1992).

92KRA Kragl, U., "Reaktionstechnik biokatatischer Prozesse am Beispiel der kontinuierlichen enzymatischen Synthese von *N*-Acetylneuraminsäure," thesis, Universität Bonn (1992).

93BES/REB Besson, V., Rebeille, F., Neuberger, M., Douce, R., Cossins, E. A., Biochem. J. **292**, 425 (1993).

93BLI/MAR Blinkovsky, A. M., Markaryan, A. N., Enzyme Microb. Technol. **15**, 965 (1993).

93BOH/HUT Bohmhammel, K., Hüttl, R., Pritzkat, K., Wolf, G., Thermochim. Acta **217**, 1 (1993).

93GOL/TEW Goldberg, R. N., Tewari, Y. B., Bell, D., Fazio, K., Anderson, E., J. Phys. Chem. Ref. Data **22**, 515 (1993).

93HUT/BOH Hüttl, R., Bohmhammel, K., Pritzkat, K., Wolf, G., Thermochim. Acta **229**, 205 (1993).

93SHI/CHE Shieh, W.-R., Chen, C.-S., J. Biol. Chem. **268**, 3487 (1993).

94CHI/KIR Chien, C., Kirollos, S. K., Linderman, R. J., Dauterman, W. C., Biochim. Biophys. Acta **1204**, 175 (1994).

94LEU/COO Leu, L.-S., Cook, P. F., Biochemistry **33**, 2667 (1994).

94NOE/COL Noeldner, P. K.-M., Coleman, M. J., Faulks, R., Oliver, R. P., Physiol. Mol. Plant Pathol. **45**, 281 (1994).

95BIS/KRA Biselli, M., Kragl, U., Wandrey, C., in *Enzyme Catalysis in Organic Synthesis*; K. Drauz and H. Waldmann, eds.; VCH, Waldheim (1995), pp. 89–155.

95CHE/ARM Chen, J., Armstrong, R. N., Chem. Res. Toxicol. **8**, 580 (1995).

95GOL/TEW Goldberg, R. N., Tewari, Y. B., J. Phys. Chem. Ref. Data **24**, 1669 (1995).

95HUT/BOH Hüttl, R., Bohmhammel, K., Wolf, G., Oehmgen, R., Thermochim. Acta **250**. 1 (1995).

95JUS/KOT Juszkiewicz, A., Kot, M., Leszko, M., Zaborska, W., Thermochim. Acta **249**, 301 (1995).

95KAM/JUR Kamp, G., Juretschke, H.-P., Thiel, U., Englisch, H., J. Comp. Physiol. B **165**, 143 (1995).

95KOZ/TOM Kozlowski, M. C., Tom, N. J., Seto, C. T., Sefler, A. M., Bartlett, P. A., J. Am. Chem. Soc. **117**, 2128 (1995).

95LEE/WAL Lees, W. J., Walsh, C. T., J. Am. Chem. Soc. **117**, 7329 (1995).

95LIA/WAN Liang, Y., Wang, C.-X., Wu, D.-Q., Song, Z.-H., Qu, S.-S., Zou, G.-L., Gaodeng Xuexiao Huaxue Xuebao **16**, 924 (1995).

95LIA/WAN2 Liang, Y., Wang, C., Wu, D., Qu, S., Thermochim. Acta **268**, 27 (1995).

95LIU/ZEN Liu, J.-S., Zeng, X.-C., Tian, A.-M., Deng, Y., Thermochim. Acta **253**, 275 (1995).

95SCH/TRA Schmidt, P. P., Travers, F., Barman, T., Biochemistry **34**, 824 (1995).

95TEW/SCH Tewari, Y. B., Schantz, M. M., Pandey, P. C., Rekharsky, M. V., Goldberg, R. N., J. Phys. Chem. **99**, 1594 (1995).

95WIS/KUS Wiseman, R. W., Kushmerick, M. J., J. Biol. Chem. **270**, 12428 (1995).

96ARA/RUZ Arabshahi, A., Ruzicka, F. J., Geeganage, S., Frey, P. A., Biochemistry **35**, 3426 (1996).

96HIR/MAY Hirata, H., Mayama, M., Kasahara, A., Yanagishita, H., Sugiura, M., Nihon Yukagakkaishi **45**, 761 (1996).

96LI/ZHA Li, Y., Zhang, Y., Yan, H., J. Biol. Chem. **271**, 28038 (1996).

96LIA/WAN Liang, Y., Wang, C.-X., Wu, D.-Q., Qu, S.-S., Acta Chimica Sinica **54**, 38, 1996.

96OES/SCH Oesterhelt, C., Schnarrenberger, C., Gross, W., Plant Sci. **121**, 19 (1996).

96PRO/GRO Prosselkov, P. V., Gross, W., Igamberdiev, A. U., Schnarrenberger, C., Physiol. Plant. **98**, 753 (1996).

96TEW/GOL Tewari, Y. B., Goldberg, R. N., J. Chem. Thermodyn. **28**, 1127 (1996).

96TEW/SCH Tewari, Y. B., Schantz, M. M., Rekharsky, M. V., Goldberg, R. N., J. Chem. Thermodyn. **28**, 171 (1996).

97CHA Chamberlin, M. E., J. Exp. Biol. **200**, 2789 (1997).

97CON/DEL Converti, A., Del Borghi, M., Enzyme Microb. Technol. **21**, 511 (1997).

97DEJ/ROC Déjardin, A., Rochat, C., Boutin, J.-P., Planta **201**, 128 (1997).

97HAN/KLE Hanschmann, H., Kleber, H.-P., Biochim. Biophys. Acta **1337**, 133 (1997).

97KAS/TEW Kast, P., Tewari, Y. B., Wiest, O., Hilvert, D., Houk, K. N., Goldberg, R. N., J. Phys. Chem. B **101**, 10976 (1997).

97LIA/WU Liang, Y., Wu, Y., Li, D., Wang, C., Liu, Y., Qu, S., Zou, G., Thermochim. Acta **307**, 149 (1997).

97PES/PRI Pestlin, S., Prinz, D., Starr, J. N., Reilly, P. J., Biotechnol. Bioeng. **56**, 9 (1997).

97SAL/GOD Salagnad, C., Gödde, A., Ernst, B., Kragl, U., Biotechnol. Prog. **13**, 810 (1997).

97STA/SUA Staples, J. F., Suarez, R. K., J. Exp. Biol. **200**, 1247 (1997).

97TEW/GOL Tewari, Y. B., Goldberg, R. N., Sato, M., Carbohyd. Res. **301**, 11 (1997).

97YOR/ISH Yorifuji, T., Ishihara, T., Naka, T., Kondo, S., Shimizu, E., J. Biochem. (Tokyo) **122**, 537 (1997).

98CON/DEL Converti, A., Del Borghi, M., Bioprocess Eng. **18**, 27 (1998).

98DIE/STR Diender, M. B., Straathof, A. J. J., van der Wielen, L. A. M., Ras, C., Heijnen, J. J., J. Mol. Catal. B: Enzymatic **5**, 249 (1998).

98KIM/VOE Kim, K.-H., Voelker, D. R., Flocco, M. T., Carman, G. M., J. Biol. Chem. **273**, 6844 (1998).

98KIS/TEW Kishore, N., Tewari, Y. B., Akers, D. L., Goldberg, R. N., Miles, E. W., Biophys. Chem. **73**, 265 (1998).

98KIS/TEW2 Kishore, N., Tewari, Y. B., Goldberg, R. N., J. Chem. Thermodyn. **30**, 1373 (1998).

98LAE/EIS Laempe, D., Eisenreich, W., Bacher, A., Fuchs, G., Eur. J. Biochem. **255**, 618 (1998).

98LOV/LAU Loverix, S., Laus, G., Martins, J. C., Wyns, L., Steyaert, J., Eur. J. Biochem. **257**, 286 (1998).

98TEW Tewari, Y. B., J. Chem. Eng. Data **43**, 750 (1998).

98TEW/CHE Tewari, Y. B., Chen, J., Holden, M. J., Houk, K. N., Goldberg, R. N., J. Phys. Chem. B **102**, 8634 (1998).

98TEW/KIS Tewari, Y. B., Kishore, N., Goldberg, R. N., Luong, T. N., J. Chem. Thermodyn. **30**, 777 (1998).

98THO/JOR Thompson, J. E., Jordan, D. B., Anal. Biochem. **256**, 7 (1998).

99HUT/OEH Hüttl, R., Oehlschläger, K., Wolf, G., Thermochim. Acta **325**, 1 (1999).

99KIS/HOL Kishore, N., Holden, M. J., Tewari, Y. B., Goldberg, R. N., J. Chem. Thermodyn. **31**, 211 (1999).

99KIS/TEW Kishore, N., Tewari, Y. B., Goldberg, R. N., J. Chem. Thermodyn. (in press).

99TEW/SCH Tewari, Y. B., Schantz, M. M., Vanderah, D. J., J. Chem. Eng. Data **44**, 641 (1999).