

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

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

Robert N. Goldberg<sup>a)</sup>

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Received February 18, 1999; final revision received May 4, 1999

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

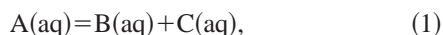
This paper serves to update a series of reviews<sup>1-5</sup> on the thermodynamics of enzyme-catalyzed reactions. These reviews, which were published during the years 1993-1995, deal with the thermodynamics of the reactions catalyzed by the six classes of enzymes classified by the Nomenclature Committee of the International Union of Biochemistry:<sup>6</sup> oxidoreductases,<sup>1</sup> transferases,<sup>2</sup> hydrolases,<sup>3</sup> lyases,<sup>4</sup> isomerases,<sup>5</sup> and ligases.<sup>5</sup> 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,<sup>1-5</sup> 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<sup>1-5</sup> 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  $\Delta_r H$  (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.<sup>7</sup> 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<sup>8,9</sup> has used data given in the previous reviews<sup>1-5</sup> 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<sup>10</sup> 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.<sup>1-5</sup> 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.<sup>1</sup> 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



$K_c = c(B)c(C)/\{c(A)c^\circ\}$ ,  $K_m = m(B)m(C)/\{m(A)m^\circ\}$ , and  $K_x = x(B)x(C)/x(A)$ . Here,  $c$ ,  $m$ , and  $x$  are, respectively, concentration, molality, and mole fraction,  $c^\circ = 1 \text{ mol dm}^{-3}$ , and  $m^\circ = 1 \text{ mol kg}^{-1}$ . 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.<sup>11-21</sup> 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

The author thanks Dr. Yadu B. Tewari for his comments on this article and Dr. David Vanderah for his help with some aspects of chemical nomenclature. Continuing discussions with Dr. Robert A. Alberty on various aspects of biochemical thermodynamics have been very helpful.

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

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



<i>T</i> /K	<i>P</i> /MPa	pH	<i>K</i> '
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

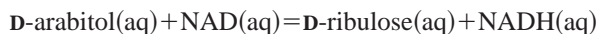
Buffer: Tris (0.1 mol dm<sup>-3</sup>) + HCl

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)



<i>T</i> /K	pH	<i>K</i> '
298.15	7.0	0.0008

Reference: 89SCH/GIF

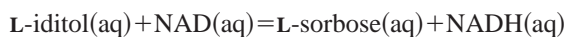
Method: spectrophotometry

Buffer: potassium phosphate (0.10 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: C

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



<i>T</i> /K	pH	<i>I</i> <sub>m</sub>	<i>K</i> '
		mol·kg <sup>-1</sup>	
298.15	7.58	0.191	0.186

Reference: 96TEW/GOL

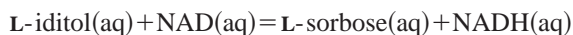
Method: HPLC and spectrophotometry

Buffer: phosphate

pH: 7.58

Evaluation: A

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



<i>T</i> /K	pH	<i>I</i> <sub>m</sub>	$\Delta_r H$ (cal)
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
298.15	7.39	0.215	-10.5

Reference: 96TEW/GOL

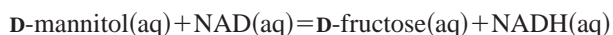
Method: calorimetry

Buffer: phosphate

pH: 7.39

Evaluation: A

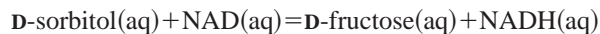
Tewari and Goldberg also calculated  $K = 2.02 \cdot 10^{-9}$  and  $\Delta_r H^\circ = 14.7 \text{ kJ mol}^{-1}$  at *T*=298.15 K and *I*=0 for the reference reaction: L-iditol(aq) + NAD<sup>-</sup>(aq) = L-sorbose(aq) + NADH<sup>2-</sup>(aq) + H<sup>+</sup>(aq).



<i>T</i> /K	pH	<i>K</i> '
298.15	7.0	0.045

Reference: 89SCH/GIF  
 Method: spectrophotometry  
 Buffer: potassium phosphate (0.10 mol dm<sup>-3</sup>)  
 pH: 7.0  
 Evaluation: C

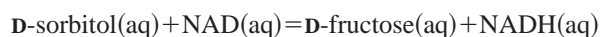
Schneider and Giffhorn reported  $K'c(\text{H}^+)/c^\circ = 4.5 \cdot 10^{-9}$  at pH=7.0. The apparent equilibrium constant given here was calculated from this result.



<i>T</i> /K	pH	<i>K'</i>
298.15	7.0	0.0058

Reference: 89SCH/GIF  
 Method: spectrophotometry  
 Buffer: potassium phosphate (0.10 mol dm<sup>-3</sup>)  
 pH: 7.0  
 Evaluation: C

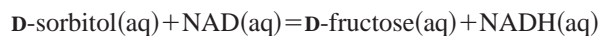
Schneider and Giffhorn reported  $K'c(\text{H}^+)/c^\circ = 5.8 \cdot 10^{-10}$  at pH=7.0. The apparent equilibrium constant given here was calculated from this result.



<i>T</i> /K	pH	<i>I<sub>m</sub></i>	
		mol·kg <sup>-1</sup>	<i>K'</i>
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  $\Delta_r H^\circ = 21.3 \text{ kJ mol}^{-1}$  at  $T = 298.15 \text{ K}$  and  $I = 0$  for the reference reaction: **D-sorbitol(aq) + NAD<sup>-</sup>(aq) = D-fructose(aq) + NADH<sup>2-</sup>(aq) + H<sup>+</sup>(aq).**

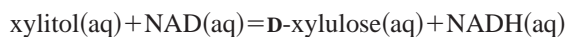


<i>T</i> /K	pH	<i>I<sub>m</sub></i>	
		mol·kg <sup>-1</sup>	$\Delta_r H(\text{cal})$ kJ·mol <sup>-1</sup>
298.15	7.55	0.217	-17.1

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

Tewari and Goldberg also calculated  $K = 9.0 \cdot 10^{-10}$  and  $\Delta_r H^\circ = 21.3 \text{ kJ mol}^{-1}$  at  $T = 298.15 \text{ K}$  and  $I = 0$  for the refer-

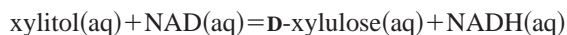
ence reaction: **D-sorbitol(aq) + NAD<sup>-</sup>(aq) = D-fructose(aq) + NADH<sup>2-</sup>(aq) + H<sup>+</sup>(aq).**



<i>T</i> /K	pH	<i>I<sub>m</sub></i>	
		mol·kg <sup>-1</sup>	<i>K'</i>
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  $\Delta_r H^\circ = 39.4 \text{ kJ mol}^{-1}$  at  $T = 298.15 \text{ K}$  and  $I = 0$  for the reference reaction: **xylitol(aq) + NAD<sup>-</sup>(aq) = D-xylulose(aq) + NADH<sup>2-</sup>(aq) + H<sup>+</sup>(aq).**

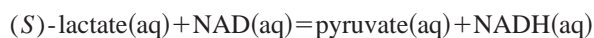


<i>T</i> /K	pH	<i>I<sub>m</sub></i>	
		mol·kg <sup>-1</sup>	$\Delta_r H(\text{cal})$ kJ·mol <sup>-1</sup>
298.15	7.43	0.218	-35.2

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

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

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



<i>T</i> /K	pH	$\Delta_r H(\text{cal})$	
		kJ·mol <sup>-1</sup>	
298.15	7.5	41.8	

Reference: 76SCH/KRI  
 Method: calorimetry  
 Buffer: phosphate (0.07 mol dm<sup>-3</sup>)  
 pH: 7.0  
 Evaluation: C

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

<i>T</i> /K	pH	<i>K'</i>
298.15	7.0	0.0033

Reference: 92KAH/SCH

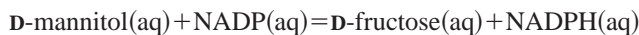
Method: spectrophotometry

Buffer: phosphate (0.1 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: C

Kahle and Schneider report  $K'c(\text{H}^+)/c^\circ = 3.3 \cdot 10^{-10}$  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)**

<i>T</i> /K	pH	<i>K'</i>
310.15	7.5	0.0917

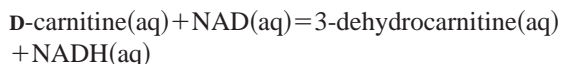
Reference: 94NOE/COL

Method: HPLC and spectrophotometry

Buffer: Tris (0.020 mol dm<sup>-3</sup>) + HCl

pH: 7.5

Evaluation: B

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

<i>T</i> /K	pH	<i>K'</i>
295.15	8.0	0.00022
295.15	9.0	0.0022

Reference: 97HAN/KLE

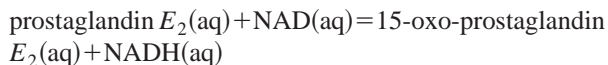
Method: spectrophotometry and HPLC

Buffer: Tris (0.05 mol dm<sup>-3</sup>) + HCl

pH: 8.0–9.0

Evaluation: B

Hanschmann and Kleber report  $K'c(\text{H}^+)/c^\circ = 2.2 \cdot 10^{-12}$  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<sup>+</sup>) (EC 1.1.1.141)**

<i>T</i> /K	pH	<i>K'</i>
298.15	7.0	$1.77 \cdot 10^2$
298.15	8.0	$1.77 \cdot 10^3$

Reference: 75SCH/GRE

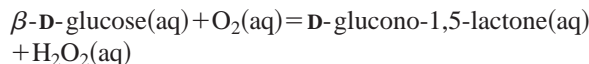
Method: spectrophotometry

Buffer: Tris (0.1 mol dm<sup>-3</sup>)

pH: 7.0–8.0

Evaluation: C

This approximate result was calculated from kinetic data. Schlegel and Greep reported that  $K'c(\text{H}^+)/c^\circ = 1.77 \cdot 10^{-5}$  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)**

<i>T</i> /K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
298.15	6.86	-125

Reference: 93BOH/HUT

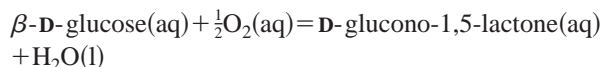
Method: calorimetry

Buffer: phosphate (0.1 mol dm<sup>-3</sup>)

pH: 6.86

Evaluation: A

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



<i>T</i> /K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
300.15	7.0	-207.1

Reference: 76SCH/KRI

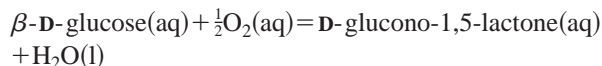
Method: calorimetry

Buffer: phosphate (0.066 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: C

Catalase (EC 1.11.1.6) was also present.



<i>T</i> /K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
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)**

<i>T</i> /K	pH	$\Delta_r H$ (cal)
		$\text{kJ}\cdot\text{mol}^{-1}$
303.15	7.0	-114

Reference: 78MCG/BRO

Method: calorimetry

Buffer: phosphate ( $0.067 \text{ mol dm}^{-3}$ )

pH: 7.0

Evaluation: B



<i>T</i> /K	pH	$\Delta_r H$ (cal)
		$\text{kJ}\cdot\text{mol}^{-1}$
303.15	7.0	-214

Reference: 78MCG/BRO

Method: calorimetry

Buffer: phosphate ( $0.067 \text{ mol dm}^{-3}$ )

pH: 7.0

Evaluation: B

Catalase (EC 1.11.1.6) was also present.



<i>T</i> /K	pH	$\Delta_r H$ (cal)
		$\text{kJ}\cdot\text{mol}^{-1}$
303.15	6.9	-153.4

Reference: 82REH/YOU

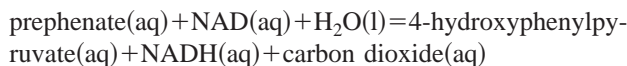
Method: calorimetry

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)**

<i>T</i> /K	pH	$I_m$	$\Delta_r H$ (cal)
		$\text{mol}\cdot\text{kg}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$
298.15	6.98	0.32	-79.0

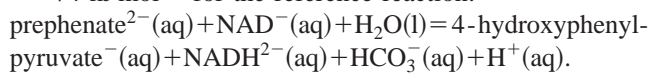
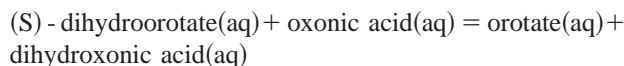
Reference: 99KIS/HOL

Method: calorimetry

Buffer: phosphate

pH: 6.98

Evaluation: A

Kishore *et al.* calculated  $\Delta_r H^\circ (T=298.15 \text{ K}, I=0)$  $= -74 \text{ kJ mol}^{-1}$  for the reference reaction:**4.11. Enzyme: dihydroorotate dehydrogenase (1.3.99.11)**

<i>T</i> /K	pH	$K'$
298.15	7.0	0.040

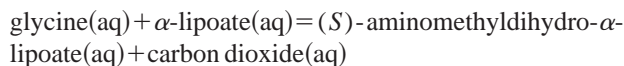
Reference: 98THO/JOR

Method: spectrophotometry

Buffer: sodium phosphate ( $0.1 \text{ mol dm}^{-3}$ )

pH: 7.0

Evaluation: B

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

<i>T</i> /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  $0.25 \text{ mol dm}^{-3}$ .



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

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

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
313.15	7.0	0.001

Reference: 64ROS/RAP

Method: spectrophotometry

Buffer: phosphate (0.125 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: C

Few details are given in this study.

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

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
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<sup>-3</sup>) and Tris (0.1 mol dm<sup>-3</sup>)

pH: 7.0–8.47

Evaluation: A

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

urate(aq)+ $\frac{1}{2}$ O<sub>2</sub>(aq)+2 H<sub>2</sub>O(l)=allantoin(aq)+carbon  
dioxide(aq)

<i>T</i> /K	pH	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
303.15	9.0	-149.6

Reference: 77REH/JAN

Method: calorimetry

Buffer: Tris (0.02 mol dm<sup>-3</sup>) + 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)

<i>T</i> /K	pH	<i>c</i> (MgCl <sub>2</sub> ) mol·dm <sup>-3</sup>	<i>I</i> <sub>c</sub> mol·dm <sup>-3</sup>	<i>K'</i>
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

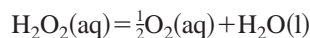
Buffer: potassium phosphate (0.050 mol dm<sup>-3</sup>) or sodium  
pyrophosphate (0.030 mol dm<sup>-3</sup>)

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<sup>-</sup>(aq) + NAD<sup>-</sup>(aq) =  $\alpha$ -lipoate<sup>-</sup>(aq) + NADH<sup>2-</sup>(aq) + H<sup>+</sup>(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)



T/K	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
298.15	-100.4

Reference: 72NEL/KIE

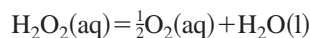
Method: calorimetry

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).



T/K	pH	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
298.15	7.0	-83.7

Reference: 95LIA/WAN

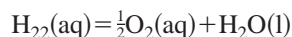
Method: calorimetry

Buffer: phosphate (0.067 mol dm<sup>-3</sup>)

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).



T/K	pH	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
298.15	7.0	-88.88

Reference: 97LIA/WU

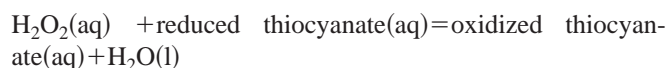
Method: calorimetry

Buffer: phosphate

pH: 7.0

Evaluation: B

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



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

Reference: 86PRU/TEN

Method: enzymatic assay and chemical analysis

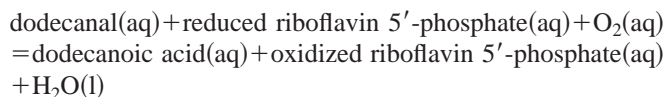
Buffer: phosphate

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:  $\text{H}_2\text{O}_2(\text{aq}) + \text{SCN}^-(\text{aq}) = \text{OSCN}^-(\text{aq}) + \text{H}_2\text{O}(\text{l})$ .

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



T/K	pH	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
280.15	7.0	-350
298.15	7.0	-308

Reference: 75MAN/LAN

Method: calorimetry

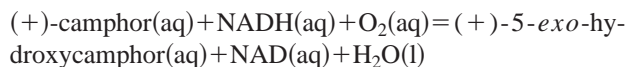
Buffer: potassium phosphate (0.15 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: C

Light is emitted by this reaction.

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



T/K	pH	$\Delta_r H$ (cal) kJ·mol <sup>-1</sup>
298.15	7.4	-405.8

Reference: 69PET/MCK

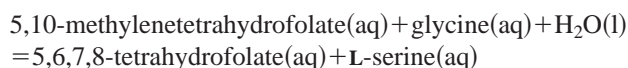
Method: calorimetry

Buffer: Tris+HCl

pH: 7.4

Evaluation: B

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



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<sub>2</sub>O(l)  
= 5,6,7,8-tetrahydrofolate(aq) + L-serine(aq)

<i>T</i> /K	pH	<i>K</i> '
310.15	7.4	0.067

Reference: 93BES/REB

Method: radioactivity

Buffer: KH<sub>2</sub>PO<sub>4</sub> (0.020 mol dm<sup>-3</sup>)

pH: 7.4

Evaluation: B

tetraglutamyl-5,10-methylenetetrahydrofolate(aq)  
+ glycine(aq) + H<sub>2</sub>O(l) = tetraglutamyl-5,6,7,8-tetrahydro-  
folate(aq) + L-serine(aq)

<i>T</i> /K	pH	<i>K</i> '
310.15	7.4	0.063

Reference: 93BES/REB

Method: radioactivity

Buffer: KH<sub>2</sub>PO<sub>4</sub> (0.020 mol dm<sup>-3</sup>)

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)

<i>T</i> /K	pH	<i>K</i> '
298.15	6.0	15

Reference: 94LEU/COO

Method: spectrophotometry

Buffer: Mes (0.1 mol dm<sup>-3</sup>)

pH: 6.0

Evaluation: A

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

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

<i>T</i> /K	pH	Buffer	<i>K</i> '
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<sup>-3</sup>) + NaOH} and {Ches (0.050  
mol dm<sup>-3</sup>) + NaOH}

pH: 7.0–9.4

Cofactor(s): MgCl<sub>2</sub>

Evaluation: B

#### 4.23. Enzyme: cyclomalto-dextrin glucanotransferase (EC 2.4.1.19)

G<sub>*u*</sub>(aq) = cyclomaltohexaose(aq) + G<sub>(*u*-6)</sub>(aq)

<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
311.15	6.5	0.0134

Reference: 50PAZ

Method: HPLC

Buffer: NaCN + NaC<sub>2</sub>H<sub>3</sub>O<sub>2</sub>

pH: 6.5

Evaluation: A

G<sub>1</sub> represents D-glucose and G<sub>*n*</sub> (*n* is a positive integer) represents a linear maltodextrin; *u* is an integer ≥ 7. The result given here is based upon Tewari and Goldberg's recalculation [97TEW/GOL] of Pazur's original data.

G<sub>*u*</sub>(aq) = cyclomaltohexaose(aq) + G<sub>(*u*-6)</sub>(aq)

<i>T</i> /K	pH	<i>K</i> ' <sub><i>m</i></sub>
329.6	5.55	0.0229

Reference: 97TEW/GOL

Method: HPLC

Buffer: phosphate

pH: 5.55

Evaluation: A

G<sub>1</sub> represents D-glucose and G<sub>*n*</sub> (*n* is a positive integer) represents a linear maltodextrin; *u* is an integer ≥ 7.

G<sub>*v*</sub>(aq) = cyclomaltoheptaose(aq) + G<sub>(*v*-7)</sub>(aq)

<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
311.15	6.5	0.0334

Reference: 50PAZ

Method: HPLC

Buffer: NaCN + NaC<sub>2</sub>H<sub>3</sub>O<sub>2</sub>

pH: 6.5

Evaluation: A

G<sub>1</sub> represents D-glucose and G<sub>*n*</sub> (*n* is a positive integer) represents a linear maltodextrin; *v* is an integer ≥ 8. The result given here is based upon Tewari and Goldberg's recalculation [97TEW/GOL] of Pazur's original data.

G<sub>*v*</sub>(aq) = cyclomaltoheptaose(aq) + G<sub>(*v*-7)</sub>(aq)

<i>T</i> /K	pH	<i>K</i> ' <sub><i>m</i></sub>
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  $\geq 8$ .



$T/\text{K}$	pH	$K'_c$
311.15	6.5	0.0194

Reference: 50PAZ

Method: HPLC

Buffer: NaCN + NaC<sub>2</sub>H<sub>3</sub>O<sub>2</sub>

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.



$T/\text{K}$	pH	$K'_m$
329.6	5.55	0.0103

Reference: 97TEW/GOL

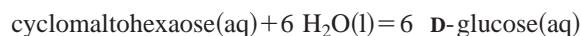
Method: HPLC

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  $\geq 9$ .



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

Reference: 97TEW/GOL

Method: calorimetry

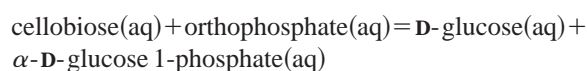
Buffer: KH<sub>2</sub>PO<sub>4</sub> (0.10 mol kg<sup>-1</sup>)

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)



$T/\text{K}$	pH	$K'$
310.15	7.0	0.23

Reference: 61ALE

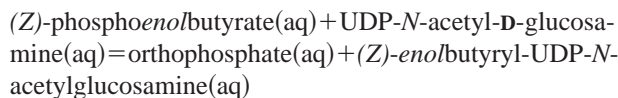
Method: enzymatic assay

Buffer: barbital (0.0075 mol dm<sup>-3</sup>) + acetate

pH: 7.0

Evaluation: B

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



$T/\text{K}$	pH	$K'$
298.15	8.0	65

Reference: 95LEE/WAL

Method: HPLC

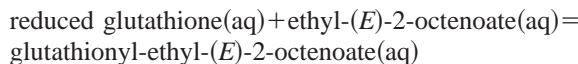
Buffer: Tris (0.050 mol dm<sup>-3</sup>)

pH: 8.0

Evaluation: C

This is an approximate result.

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



$T/\text{K}$	pH	$K'_c$
298.15	7.4	435

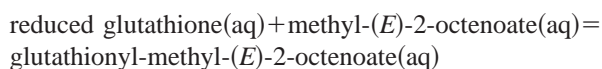
Reference: 94CHI/KIR

Method: HPLC

Buffer: phosphate (0.066 mol dm<sup>-3</sup>)

pH: 7.4

Evaluation: B



$T/\text{K}$	pH	$K'_c$
298.15	7.4	212

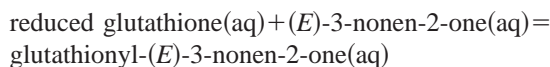
Reference: 94CHI/KIR

Method: HPLC

Buffer: phosphate (0.066 mol dm<sup>-3</sup>)

pH: 7.4

Evaluation: B



$T/\text{K}$	pH	$K'_c$
298.15	7.4	$2.6 \cdot 10^3$

Reference: 94CHI/KIR

Method: HPLC

Buffer: phosphate (0.066 mol dm<sup>-3</sup>)

pH: 7.4

Evaluation: B

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

<i>T</i> /K	pH	<i>K</i> ' <sub>c</sub>
298.15	7.4	7.1 · 10 <sup>3</sup>

Reference: 94CHI/KIR

Method: HPLC

Buffer: phosphate (0.066 mol dm<sup>-3</sup>)

pH: 7.4

Evaluation: B

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

<i>T</i> /K	pH	<i>K</i> ' <sub>c</sub>
298.15	8.0	640

Reference: 95CHE/ARM

Method: spectrophotometry

Buffer: Tris (0.1 mol dm<sup>-3</sup>)

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*'<sub>c</sub> 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>T</i> /K	pH	$\frac{I_m}{\text{mol} \cdot \text{kg}^{-1}}$	<i>K</i> '
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, Δ<sub>r</sub>*H*<sup>o</sup> = 1.9 kJ mol<sup>-1</sup>, and Δ<sub>r</sub>*S*<sup>o</sup> = -10 J K<sup>-1</sup> mol<sup>-1</sup> at *T* = 298.15 K and *I* = 0 for the reference reaction: L-aspartate<sup>-</sup>(aq) + 2-oxoglutarate<sup>2-</sup>(aq) = oxaloacetate<sup>2-</sup>(aq) + L-glutamate<sup>-</sup>(aq).

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

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

+ L-glutamate(aq)

<i>T</i> /K	pH	$\frac{I_c}{\text{mol} \cdot \text{dm}^{-3}}$	<i>K</i> '
311.15	7.0	0.25	0.68

Reference: 68BRO

Method: spectrophotometry

Buffer: phosphate (0.1 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: A

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

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

+ L-glutamate(aq)

<i>T</i> /K	pH	$\frac{I_c}{\text{mol} \cdot \text{dm}^{-3}}$	<i>K</i> '
311.15	7.0	0.25	0.68

Reference: 70BRO/KRE

Method: spectrophotometry

Buffer: phosphate (0.1 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: A

Also see Brosnan [68BRO].

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

+ L-glutamate(aq)

<i>T</i> /K	pH	$\frac{I_m}{\text{mol} \cdot \text{kg}^{-1}}$	<i>K</i> '
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 Δ<sub>r</sub>*H*<sup>o</sup> = 5.9 kJ mol<sup>-1</sup> at *T* = 298.15 K and *I* = 0 for the reference reaction:

L-alanine(aq) + 2-oxoglutarate<sup>2-</sup>(aq) = pyruvate<sup>-</sup>(aq) + L-glutamate<sup>-</sup>(aq).

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

+ L-glutamate(aq)

<i>T</i> /K	pH	$\frac{I_m}{\text{mol} \cdot \text{kg}^{-1}}$	$\frac{\Delta_r H(\text{cal})}{\text{kJ} \cdot \text{mol}^{-1}}$
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  $\Delta_r H^\circ = 5.9 \text{ kJ mol}^{-1}$  at  $T=298.15 \text{ K}$  and  $I=0$  for the reference reaction: L-alanine(aq)+2-oxoglutarate<sup>2-</sup>(aq)=pyruvate<sup>-</sup>(aq)+L-glutamate<sup>-</sup>(aq).

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

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

T/K	pH	$I_m$	$K'$
		mol·kg <sup>-1</sup>	
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  $\Delta_r H^\circ = 9.5 \text{ kJ mol}^{-1}$  at  $T=298.15 \text{ K}$  and  $I=0$  for the reference reaction: L-phenylalanine(aq)+2-oxoglutarate<sup>2-</sup>(aq)=phenylpyruvate<sup>-</sup>(aq)+L-glutamate<sup>-</sup>(aq).

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

T/K	pH	$I_m$	$\Delta_r H^\circ$ (cal)
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
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  $\Delta_r H^\circ = 9.5 \text{ kJ mol}^{-1}$  at  $T=298.15 \text{ K}$  and  $I=0$  for the reference reaction: L-phenylalanine(aq)+2-oxoglutarate<sup>2-</sup>(aq)=phenylpyruvate<sup>-</sup>(aq)+L-glutamate<sup>-</sup>(aq).

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

T/K	pH	$I_m$	$K'$
		mol·kg <sup>-1</sup>	
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  $\Delta_r H^\circ = 10.1 \text{ kJ mol}^{-1}$  at  $T=298.15 \text{ K}$  and  $I=0$  for the reference reaction: L-tyrosine(aq)+2-oxoglutarate<sup>2-</sup>(aq)=4-hydroxyphenylpyruvate<sup>-</sup>(aq)+L-glutamate<sup>-</sup>(aq).

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

T/K	pH	$I_m$	$\Delta_r H^\circ$ (cal)
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
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  $\Delta_r H^\circ = 10.1 \text{ kJ mol}^{-1}$  at  $T=298.15 \text{ K}$  and  $I=0$  for the reference reaction: L-tyrosine(aq)+2-oxoglutarate<sup>2-</sup>(aq)=4-hydroxyphenylpyruvate<sup>-</sup>(aq)+L-glutamate<sup>-</sup>(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<sup>-3</sup>) + HCl

pH: 9.0

Evaluation: B

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

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

<i>T</i> /K	pH	<i>K</i> '
303.15	9.5	0.2

Reference: 98KIM/VOE

Method: radioactivity

Buffer: glycine (0.067 mol dm<sup>-3</sup>) + NaOH

pH: 9.5

Cofactor(s): MgSO<sub>4</sub> (0.010 mol dm<sup>-3</sup>)

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)

<i>T</i> /K	pH	Cosolvent	<i>K</i> '
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<sup>-3</sup>)

pH: 7.5

Cofactor(s): Mg<sup>2+</sup> (0.001 mol dm<sup>-3</sup>)

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)

<i>T</i> /K	pH	<i>K</i> '
296.15	7.0	34.3

Reference: 95WIS/KUS

Method: NMR and HPLC

Buffer: Mops (0.1 mol dm<sup>-3</sup>) + Tris (0.070 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: B

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

<i>T</i> /K	pH	<i>K</i> '
298.15	7.06	3.06

Reference: 86MEY/BRO

Method: enzymatic assay

Buffer: Pipes (0.050 mol dm<sup>-3</sup>)

pH: 7.06

Cofactor(s): MgCl<sub>2</sub> (0.010 mol dm<sup>-3</sup>)

Evaluation: B

The temperature was assumed to be 298.15 K.

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

<i>T</i> /K	pH	<i>K</i> '
296.15	7.0	3.1

Reference: 95WIS/KUS

Method: NMR and HPLC

Buffer: Mops (0.1 mol dm<sup>-3</sup>) + Tris (0.070 mol dm<sup>-3</sup>)

pH: 7.0

Evaluation: B

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

ATP(aq) + L-arginine(aq) = ADP(aq) + *N*<sup>ω</sup>-phospho-L-arginine(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	7.2	17.5

Reference: 97CHA

Method: spectrophotometry

Buffer: imidazole (0.1 mol dm<sup>-3</sup>)

pH: 7.2

Cofactor(s): MgCl<sub>2</sub> (0.005 mol dm<sup>-3</sup>)

Evaluation: B

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

ATP(aq) + taurocyamine(aq) = ADP(aq) + *N*<sup>ω</sup>-phosphotaurocyamine(aq)

<i>T</i> /K	pH	<i>K</i> '
285.15	7.3	1 · 10 <sup>9</sup>

Reference: 95KAM/JUR

Method: enzymatic analysis

Buffer: Tris (0.1 mol dm<sup>-3</sup>) + HCl

pH: 7.3

Cofactor(s): magnesium acetate (0.10 mol dm<sup>-3</sup>)

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)

<i>T</i> /K	pH	<i>K</i> '
285.15	7.3	0.36

Reference: 95KAM/JUR

Method: enzymatic analysis  
 Buffer: Tris (0.1 mol dm<sup>-3</sup>) + HCl  
 pH: 7.3  
 Cofactor(s): magnesium acetate (0.060 mol dm<sup>-3</sup>)  
 Evaluation: C

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

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

T/K	pH	$c(\text{MgCl}_2)$	$K'$
		mol · dm <sup>-3</sup>	
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<sup>2+</sup>  
 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<sup>-3</sup>)  
 pH: 8.5  
 Cofactor(s): MgCl<sub>2</sub>  
 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	$c(\text{MgSO}_4)$	pMg	$K'$
			mol · dm <sup>-3</sup>		
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<sup>-3</sup>) + HCl} and {imidazole (0.1 mol dm<sup>-3</sup>) + 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  $\Delta_r H'^\circ(T=291 \text{ K}, \text{pH}=7.4, \text{pMg}=2.0) \approx -28 \text{ kJ mol}^{-1}$  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<sup>-3</sup>) and Bicine (0.095 mol · dm<sup>-3</sup>)  
 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) = dodecyl dodecanoate(sln) + H<sub>2</sub>O(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  $K_m(T=298.15 \text{ K}, I=0)=2.9 \cdot 10^6$  for the reaction: 1-dodecanol(aq) + 1-dodecanoic acid(aq) = dodecyl dodecanoate(aq) + H<sub>2</sub>O(l).

1-dodecanoic acid(sln) + (-)-menthol(sln) = (-)-menthyl dodecanoate(sln) + H<sub>2</sub>O(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<sub>2</sub>O) partition coefficients for (-)-menthol, 1-dodecanoic acid, and (-)-menthyl dodecanoate. By using a thermodynamic cycle calculation they calculated  $K_m(T=298.15 \text{ K}, I=0)=1.9 \cdot 10^5$  for the reference reaction: (-)-menthol(aq) + 1-dodecanoic acid(aq) = (-)-menthyl dodecanoate(aq) + H<sub>2</sub>O(l).

tributrylglycerol(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.

tributrylglycerol(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.

tributrylglycerol(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.

tributrylglycerol(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.

tributrylglycerol(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.

tributrylglycerol(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<sub>2</sub>O(l) = 3,4,5-trihydroxybenzoate(aq) + 1-propanol(aq)

T/K	pH	$I_m$ mol·kg <sup>-1</sup>	$K'_m$
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  
pH: 4.99–6.56  
Evaluation: A

Tewari *et al.* also calculated  $K_m = 4.37 \cdot 10^{-4}$  and  $\Delta_r H^\circ = -4.6 \text{ kJ mol}^{-1}$  at  $T = 298.15 \text{ K}$  and  $I = 0$  for the reference reaction: 3,4,5-trihydroxybenzoic acid propyl ester(aq) + H<sub>2</sub>O(l) = 3,4,5-trihydroxybenzoate<sup>-</sup>(aq) + 1-propanol(aq) + H<sup>+</sup>(aq).

3,4,5-trihydroxybenzoic acid propyl ester(aq) + H<sub>2</sub>O(l) = 3,4,5-trihydroxybenzoate(aq) + 1-propanol(aq)

T/K	pH	Buffer	$I_m$ mol·kg <sup>-1</sup>	$\Delta_r H^\circ$ kJ·mol <sup>-1</sup>
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  $K_m = 4.37 \cdot 10^{-10}$  and  $\Delta_r H^\circ = -4.6 \text{ kJ mol}^{-1}$  at  $T = 298.15 \text{ K}$  and  $I = 0$  for the reference reaction: 3,4,5-trihydroxybenzoic acid propyl ester(aq) + H<sub>2</sub>O(l) = 3,4,5-trihydroxybenzoate<sup>-</sup>(aq) + 1-propanol(aq) + H<sup>+</sup>(aq).

3,4,5-trihydroxybenzoic acid propyl ester(sln) + H<sub>2</sub>O(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  $\Delta_r H^\circ(\langle T \rangle = 301 \text{ K}) = -15.4 \text{ kJ mol}^{-1}$  from the temperature dependence of the equilibrium constant.

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

guanosine 2':3'-(cyclic)phosphate(aq) + H<sub>2</sub>O(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<sup>-3</sup>)  
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  $K'c^\circ/c(\text{H}_2\text{O}) = 0.38$  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)

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
308.15	6.0	≈ 0.95

Reference: 98LOV/LAU

Method: mass spectrometry

Buffer: imidazole (0.0125 mol dm<sup>-3</sup>)

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<sub>2</sub>O(l) = uridine 3'-monophosphate(aq)

<i>T</i> /K	pH	<i>K'</i>
298.15	5.0	440

Reference: 69ROS/HAM

Method: chromatography and radioactivity

Buffer: Tris (0.1 mol dm<sup>-3</sup>) + acetate

pH: 5.0

Evaluation: B

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

cyclomaltoheptaose(aq) + 7 H<sub>2</sub>O(l) = 7 D-glucose(aq)

<i>T</i> /K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
298.15	5.14	-48.79

Reference: 97TEW/GOL

Method: calorimetry

Buffer: KH<sub>2</sub>PO<sub>4</sub> (0.10 mol kg<sup>-1</sup>)

pH: 5.14

Evaluation: A

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

cyclomaltooctaose(aq) + 8 H<sub>2</sub>O(l) = 8 D-glucose(aq)

<i>T</i> /K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
298.15	5.15	-52.29

Reference: 97TEW/GOL

Method: calorimetry

Buffer: KH<sub>2</sub>PO<sub>4</sub> (0.10 mol kg<sup>-1</sup>)

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<sub>2</sub>O(l) = 2 D-galactose(aq)

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
318.15	4.5	≈ 1.04 · 10 <sup>3</sup>

Reference: 97PES/PRI

Method: GC+MS

Buffer: acetate (0.05 mol dm<sup>-3</sup>)

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<sub>2</sub>O(l)  
= D-glucose(aq) + D-fructose(aq)

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
318.15	4.5	372

Reference: 97PES/PRI

Method: GC+MS

Buffer: acetate (0.05 mol dm<sup>-3</sup>)

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<sub>2</sub>O(l)  
= D-glucose(aq) + lyxose(aq)

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
318.15	4.5	330

Reference: 97PES/PRI

Method: GC+MS

Buffer: acetate (0.05 mol dm<sup>-3</sup>)

pH: 4.5

Evaluation: B

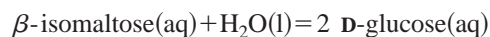
The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VII.

α-isomaltose(aq) + H<sub>2</sub>O(l) = 2 D-glucose(aq)

<i>T</i> /K	pH	<i>K'</i> <sub>c</sub>
318.15	4.5	81

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 pH: 4.5  
 Evaluation: B

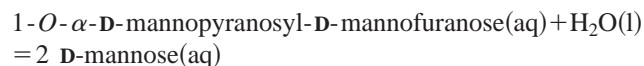
The result given here is the average of the results calculated from the concentrations given in Pestlin *et al.*'s Tables III to X.



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
318.15	4.5	65

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 pH: 4.5  
 Evaluation: B

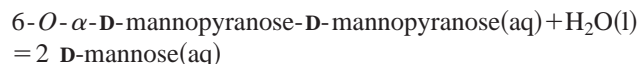
The result given here is the average of the results calculated from the concentrations given in Pestlin *et al.*'s Tables III to X.



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
318.15	4.5	1.26 · 10 <sup>3</sup>

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 pH: 4.5  
 Evaluation: B

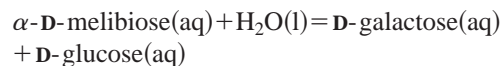
The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VIII.



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
318.15	4.5	≈ 420

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 pH: 4.5  
 Evaluation: B

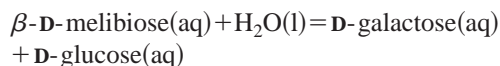
The result given here was calculated from the concentrations given in Pestlin *et al.*'s Table VIII.



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
318.15	4.5	53

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 pH: 4.5  
 Evaluation: B

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

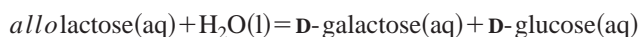


<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
318.15	4.5	40

Reference: 97PES/PRI  
 Method: GC+MS  
 Buffer: acetate (0.05 mol dm<sup>-3</sup>)  
 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)



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
310.15	7.0	45

Reference: 92ELL/SRI  
 Method: HPLC  
 Buffer: Tes (0.030 mol dm<sup>-3</sup>) + NaOH  
 pH: 7.0  
 Cofactor(s): MgCl<sub>2</sub>(0.001 mol dm<sup>-3</sup>)  
 Evaluation: A



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
310.15	7.0	152

Reference: 92ELL/SRI  
 Method: HPLC  
 Buffer: Tes (0.030 mol dm<sup>-3</sup>) + NaOH  
 pH: 7.0  
 Cofactor(s): MgCl<sub>2</sub>(0.001 mol dm<sup>-3</sup>)  
 Evaluation: A



<i>T</i> /K	pH	<i>K</i> ' <sub><i>c</i></sub>
310.15	7.0	40

Reference: 92ELL/SRI  
 Method: HPLC

Buffer: Tes (0.030 mol dm<sup>-3</sup>)+NaOH  
 pH: 7.0  
 Cofactor(s): MgCl<sub>2</sub>(0.001 mol dm<sup>-3</sup>)  
 Evaluation: A

#### 4.48. Enzyme: $\beta$ -fructofuranosidase (EC: 3.2.1.26)

sucrose(aq)+H<sub>2</sub>O(l)=D-glucose(aq)+D-fructose(aq)

T/K	pH	$\Delta_r H$ (cal)
		kJ·mol <sup>-1</sup>
298.15	4.6	-15.5

Reference: 99HUT/OEH

Method: calorimetry

Buffer: acetate (0.05 mol dm<sup>-3</sup>)

pH: 4.6

Cofactor(s): Cd<sup>2+</sup>, Zn<sup>2+</sup>, As<sup>3+</sup>, As<sup>5+</sup>, and Ag<sup>+</sup>

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<sub>2</sub>O(l)  
 =*N*-acetyl-L-phenylalanine(aq)+ethanol(aq)

T/K	pH	$I_m$	
		mol·kg <sup>-1</sup>	$K'_m$
288.15	6.09	0.11	3.55·10 <sup>3</sup>
288.15	6.29	0.11	7.98·10 <sup>3</sup>
293.15	6.17	0.11	2.27·10 <sup>3</sup>
293.15	6.39	0.13	4.28·10 <sup>3</sup>
298.15	6.19	0.12	4.04·10 <sup>3</sup>
298.15	6.44	0.13	5.29·10 <sup>3</sup>
308.15	5.98	0.11	1.63·10 <sup>3</sup>
308.15	6.23	0.12	1.99·10 <sup>3</sup>

Reference: 95TEW/SCH

Method: HPLC and GC

Buffer: phosphate

pH: 5.98–6.44

Evaluation: A

Tewari *et al.* also calculated  $K_m=1.7\cdot 10^{-3}$  and  $\Delta_r H^\circ = -3.5$  kJ mol<sup>-1</sup> at  $T=298.15$  K and  $I=0$  for the reference reaction: *N*-acetyl-L-phenylalanine ethyl ester(aq)+H<sub>2</sub>O(l)=*N*-acetyl-L-phenylalanine<sup>-</sup>(aq)+ethanol(aq)+H<sup>+</sup>(aq).

*N*-acetyl-L-phenylalanine ethyl ester(sln)+H<sub>2</sub>O(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  $\Delta_r H^\circ$  from the temperature dependence of the equilibrium constants:  $\Delta_r H^\circ(\langle T \rangle = 291$  K) = 20 kJ mol<sup>-1</sup> for the reaction in dichloromethane;  $\Delta_r H^\circ(\langle T \rangle = 291$  K) = -28 kJ mol<sup>-1</sup> for the reaction in carbon tetrachloride; and  $\Delta_r H^\circ(\langle T \rangle = 291$  K) = -26 kJ mol<sup>-1</sup> for the reaction in toluene.

*N*-acetyl-L-tryptophan ethyl ester(aq)+H<sub>2</sub>O(l)=*N*-acetyl-L-tryptophan(aq)+ethanol(aq)

T/K	pH	$I_c$	$\Delta_r H$ (cal)
		mol·dm <sup>-3</sup>	kJ·mol <sup>-1</sup>
298.15	7.5	0.1	-5.9

Reference: 71RAJ/LUM

Method: calorimetry

Buffer: phosphate (0.05 mol dm<sup>-3</sup>)

pH: 7.5

Evaluation: B

Rajender *et al.* applied buffer protonation and ionization corrections to obtain  $\Delta_r H^\circ = 3.3$  kJ mol<sup>-1</sup> for the reference reaction: *N*-acetyl-L-tryptophan ethyl ester(aq)+H<sub>2</sub>O(l)=*N*-acetyl-L-tryptophan(aq)+ethanol(aq).

*N*-acetyl-L-tyrosine ethyl ester(aq)+H<sub>2</sub>O(l)=*N*-acetyl-L-tyrosine(aq)+ethanol(aq)

T/K	pH	$\Delta_r H$ (cal)
		kJ mol <sup>-1</sup>
298.15	7.8	-48.5

Reference: 95LIU/ZEN

Method: calorimetry

Buffer: Tris

pH: 7.8  
Evaluation: B

2-propylhippurate(aq) + H<sub>2</sub>O(l) = 2-propanol(aq) + hippurate(aq)

T/K	pH	$\Delta_r H$ (cal)
		kJ mol <sup>-1</sup>
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<sub>2</sub>O(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<sub>2</sub> (0.005 mol dm<sup>-3</sup>)  
Evaluation: B

Nakanishi *et al.* reported  $K'_c \cdot c(\text{H}_2\text{O}) = 1/70$ . The apparent equilibrium constant given here was calculated from this result.

*N*-(benzyloxycarbonyl)-L-aspartyl-L-phenylalanine methyl ester(aq) + H<sub>2</sub>O(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<sub>2</sub>O(l) = L-aspartate(aq) + ammonia(aq)

T/K	pH	$I_m$	$\Delta_r H$ (cal)
		mol · kg <sup>-1</sup>	kJ · mol <sup>-1</sup>
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -26.2 \text{ kJ mol}^{-1}$  for the reference reaction:  
L-asparagine<sup>±</sup>(aq) + H<sub>2</sub>O(l) = L-aspartate<sup>-</sup>(aq) + NH<sub>4</sub><sup>+</sup>(aq).

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

L-glutamine(aq) + H<sub>2</sub>O(l) = L-glutamate(aq) + ammonia(aq)

T/K	pH	$I_m$	$\Delta_r H$ (cal)
		mol · kg <sup>-1</sup>	kJ · mol <sup>-1</sup>
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -25.2 \text{ kJ mol}^{-1}$  for the reference reaction:  
L-glutamine<sup>±</sup>(aq) + H<sub>2</sub>O(l) = L-glutamate<sup>-</sup>(aq) + NH<sub>4</sub><sup>+</sup>(aq).

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

ammonium carbamate(aq) + H<sub>2</sub>O(l) = 2 ammonia(aq) + carbon dioxide(aq)

T/K	pH	Buffer	$\Delta_r H$ (cal)
			kJ · mol <sup>-1</sup>
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<sub>2</sub>O(l) = 2 ammonia(aq) + carbon dioxide(aq)

T/K	pH	$\Delta_r H$ (cal)
		kJ · mol <sup>-1</sup>
300.15	7.0	-7.1
300.15	8.0	-8.4

Reference: 76SCH/KRI

Method: calorimetry  
 Buffer: Tris (0.05 mol dm<sup>-3</sup>)  
 pH: 7.0  
 Evaluation: C

urea(aq) + 2 H<sub>2</sub>O(l) = 2 ammonia(aq) + carbon dioxide(aq)

T/K	pH	Buffer	$\Delta_r H(\text{cal})$
			kJ·mol <sup>-1</sup>
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<sub>2</sub>O(l) = 2 ammonia(aq) + carbon dioxide(aq)

T/K	pH	$I_c$	$\Delta_r H(\text{cal})$
		mol·dm <sup>-3</sup>	kJ·mol <sup>-1</sup>
298.15	7.0	0.07	-59.6

Reference: 95JUS/KOT  
 Method: calorimetry  
 Buffer: phosphate (0.022 mol dm<sup>-3</sup>)  
 pH: 7.0  
 Evaluation: C

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

amoxicillin(aq) + H<sub>2</sub>O(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<sub>2</sub>HPO<sub>4</sub> (0.1 mol dm<sup>-3</sup>) + 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<sub>2</sub>O(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<sub>2</sub>O(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<sub>2</sub>O(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)

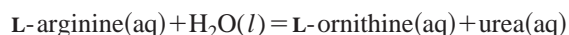
L-arginine(aq) + H<sub>2</sub>O(l) = L-ornithine(aq) + urea(aq)

T/K	pH	$\Delta_r H(\text{cal})$
		kJ·mol <sup>-1</sup>
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].





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

Reference: 95LIU/ZEN

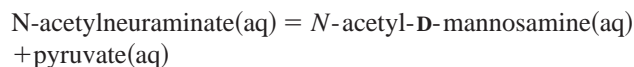
Method: calorimetry

Buffer: glycine+NaOH

pH: 9.5

Evaluation: B

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



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

Reference: 62BRU/JOU

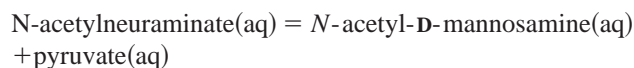
Method: radioactivity and spectrophotometry

Buffer: phosphate ( $0.1 \text{ mol dm}^{-3}$ )

pH: 7.2

Evaluation: A

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



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

Reference: 84UCH/TSU

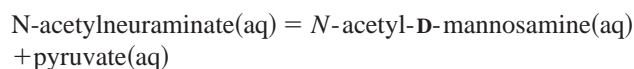
Method: spectrophotometry

Buffer: phosphate ( $0.050 \text{ mol dm}^{-3}$ )

pH: 7.7

Evaluation: B

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



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

Reference: 91KRA/GYG

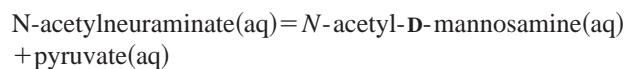
Method: HPLC

Buffer: none

pH: 7.5

Evaluation: A

Also see Kragel's thesis [92KRA].



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

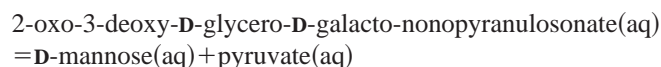
Method: HPLC

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  $\Delta_r H'^\circ(\langle T \rangle = 298 \text{ K}, \text{pH} = 7.5) = 47.8 \text{ kJ mol}^{-1}$  for this biochemical reaction from the temperature dependency of the apparent equilibrium constant. Also see Kragel *et al.* [91KRA/GYG].



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

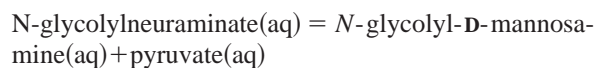
Reference: 97SAL/GOD

Method: HPLC

Buffer: none

pH: 7.5

Evaluation: B



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

Reference: 62BRU/JOU

Method: radioactivity and spectrophotometry

Buffer: phosphate ( $0.1 \text{ mol dm}^{-3}$ )

pH: 7.2

Evaluation: A

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



T/K	pH	$I_m$	$\Delta_r H$ (cal)
		$\text{mol}\cdot\text{kg}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -144 \text{ kJ mol}^{-1}$  for the reference reaction:  
 $\text{chorismate}^{2-}(\text{aq}) = \text{pyruvate}^{-}(\text{aq}) + 4\text{-hydroxybenzoate}^{-}(\text{aq})$ .

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

cyclohexa-1,5-diene-1-carboxyl-CoA(aq) + H<sub>2</sub>O(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<sup>-3</sup>)  
 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)

T/K	pH	$\Delta_r H(\text{cal})$
		kJ·mol <sup>-1</sup>
298.15	7.5	-33.8

Reference: 85WIE/HIN  
 Method: calorimetry and spectrophotometry  
 Buffer: sodium diphosphate (0.1 mol dm<sup>-3</sup>)  
 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  $\Delta_r H(\text{cal})$  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)

T/K	pH	$I_m$	K' <sub>m</sub>
		mol·kg <sup>-1</sup>	
298.15	7.54	0.37	1.2·10 <sup>4</sup>

Reference: 98KIS/TEW

Method: HPLC  
 Buffer: phosphate  
 pH: 7.54  
 Evaluation: A

Kishore *et al.* calculated  $K_m(T=298.15 \text{ K}, I=0) = 1.2 \cdot 10^{-4}$  for the reference reaction: indole<sup>0</sup>(aq) + D-glyceraldehyde 3-phosphate<sup>2-</sup>(aq) = 1-(indol-3-yl)glycerol 3-phosphate<sup>2-</sup>(aq).

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

T/K	pH	$I_m$	$\Delta_r H(\text{cal})$
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
298.15	7.26	0.37	-46.9

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

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

indole(aq) + L-serine(aq) = L-tryptophan(aq) + H<sub>2</sub>O(l)

T/K	pH	$I_m$	$\Delta_r H(\text{cal})$
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -74.3 \text{ kJ mol}^{-1}$  for the reference reaction: indole<sup>0</sup>(aq) + L-serine<sup>±</sup>(aq) = L-tryptophan<sup>±</sup>(aq) + H<sub>2</sub>O(l).

1-(indol-3-yl)glycerol 3-phosphate(aq) + L-serine(aq) = L-tryptophan(aq) + D-glyceraldehyde 3-phosphate(aq) + H<sub>2</sub>O(l)

T/K	pH	$\Delta_r H(\text{cal})$
		kJ·mol <sup>-1</sup>
298.15	7.5	-34

Reference: 85WIE/HIN  
 Method: calorimetry and spectrophotometry  
 Buffer: sodium diphosphate (0.1 mol dm<sup>-3</sup>)  
 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<sub>2</sub>O(l)

T/K	pH	$I_m$	$\Delta_r H(\text{cal})$
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
298.15	7.57	0.36	-27.8

Reference: 98KIS/TEW

Method: calorimetry

Buffer: phosphate

pH: 7.57

Evaluation: A

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

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

T/K	pH	$I_m$	$\Delta_r H(\text{cal})$
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -12.2 \text{ kJ mol}^{-1}$  for the reference reaction: L-serine<sup>±</sup>(aq) = pyruvate<sup>-</sup>(aq) + NH<sub>4</sub><sup>+</sup>(aq).

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

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

T/K	pH	$I_m$	$\Delta_r H(\text{cal})$
		mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
298.15	7.17	0.35	-127.0

Reference: 99KIS/HOL

Method: calorimetry

Buffer: phosphate

pH: 7.17

Evaluation: A

Kishore *et al.* calculated  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -126 \text{ kJ mol}^{-1}$  for the reference reaction: prephenate<sup>2-</sup>(aq) = phenylpyruvate<sup>-</sup>(aq) + HCO<sub>3</sub><sup>-</sup>(aq).

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

chorismate(aq) + ammonia(aq) = 4-amino-4-deoxychorismate(aq) + H<sub>2</sub>O(l)

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

Reference: 91AND/KAT

Method: HPLC

Buffer: Tris (0.050 mol dm<sup>-3</sup>)

pH: 8.6

Cofactor(s): MgCl<sub>2</sub> (0.010 mol dm<sup>-3</sup>)

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<sup>-3</sup>)

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<sup>-3</sup>)

pH: 8.7

Evaluation: C

UDPGlucose(aq)=UDPGalactose(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	8.7	0.30

Reference: 70TSA/HOL

Method: spectrophotometry

Buffer: glycine (0.1 mol dm<sup>-3</sup>)+NaOH

pH: 8.7

Evaluation: A

UDPGlucose(aq)=UDPGalactose(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	8.7	0.29

Reference: 80FUK/OBO

Method: spectrophotometry

Buffer: glycine (0.1 mol dm<sup>-3</sup>)+NaOH

pH: 8.7

Evaluation: B

UDPGlucose(aq)=UDPGalactose(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	8.5	0.29

Reference: 96PRO/GRO

Method: spectrophotometry

Buffer: Tris (0.020 mol dm<sup>-3</sup>)+HCl

pH: 8.5

Cofactor(s): MgCl<sub>2</sub> (0.001 mol dm<sup>-3</sup>)

Evaluation: C

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

*N*-acetyl-D-glucosamine(aq)=*N*-acetyl-D-manno-samine(aq)

<i>T</i> /K	pH	<i>K</i> '
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)

<i>T</i> /K	pH	<i>K</i> '
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<sup>-3</sup>)

pH: 7.0

Cofactor(s): MgSO<sub>4</sub>

Evaluation: C

We calculate  $\Delta_r H'^\circ(\langle T \rangle = 343.15 \text{ K}, \text{pH} = 7.0) = 16.9 \text{ kJ mol}^{-1}$  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)

<i>T</i> /K	pH	buffer	<i>K</i> '
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<sup>-3</sup>) and Tris (0.025 mol dm<sup>-3</sup>)

pH: 7.0–8.0

Cofactor(s): MgCl<sub>2</sub> (0.005 mol dm<sup>-3</sup>)

Evaluation: A

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

$\alpha$ -D-glucose 1-phosphate(aq)= $\alpha$ -D-glucose 6-phosphate(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	7.0	3.7

Reference: 96OES/SCH

Method: enzymatic assay and spectrophotometry

Buffer: Tris (0.050 mol dm<sup>-3</sup>)+HCl

pH: 7.0

Cofactor(s): MgCl<sub>2</sub> (0.001 mol dm<sup>-3</sup>)

Evaluation: B

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

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

$\alpha$ -D-glucose 1-phosphate(aq)= $\alpha$ -D-glucose 6-phosphate(aq)

<i>T</i> /K	pH	<i>K</i> '
298.15	7.0	1.4

Reference: 96OES/SCH

Method: enzymatic assay and spectrophotometry

Buffer: Tris (0.050 mol dm<sup>-3</sup>)+HCl

pH: 7.0

Cofactor(s): MgCl<sub>2</sub> (0.001 mol dm<sup>-3</sup>)

Evaluation: B

Also see data given under  $\beta$ -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<sup>-3</sup>) + HCl

pH: 7.0

Cofactor(s): MgCl<sub>2</sub> (0.001 mol dm<sup>-3</sup>)

Evaluation: B

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

chorismate(aq) = prephenate(aq)

T/K	pH	buffer	$I_m$	$\Delta_r H$ (cal)
			mol·kg <sup>-1</sup>	kJ·mol <sup>-1</sup>
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  $\Delta_r H^\circ(T=298.15 \text{ K}, I=0) = -55.4 \text{ kJ mol}^{-1}$  for the reference reaction: chorismate<sup>2-</sup>(aq) = prephenate<sup>2-</sup>(aq). This study was complemented by a quantum mechanical calculation of  $\Delta_r H^\circ$  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<sup>-3</sup>)

pH: 7.5

Cofactor(s): MgCl<sub>2</sub> (0.005 mol dm<sup>-3</sup>)

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<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> (0.050 mol dm<sup>-3</sup>)

pH: 8.0

Evaluation: C

The temperature was assumed to be 298.15 K.

chorismate(aq) + ammonia(aq) = 2-amino-2-deoxyisochorismate(aq) + H<sub>2</sub>O(l)

T/K	pH	$K'$
298.15	8.0	2.67

Reference: 95KOZ/TOM

Method: HPLC

Buffer: (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> (0.050 mol dm<sup>-3</sup>)

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 <sup>a</sup>	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	2.3.1.30
<i>N</i> -acetyl-D-glucosamine	7512-17-6	5.1.3.8
<i>N</i> -acetyl-D-mannosamine	3615-17-6	4.1.3.3, 5.1.3.8
<i>N</i> -acetyl-L-methionine	65-82-7	3.5.1.14
<i>N</i> -acetylneuraminate	131-48-6	4.1.3.3
<i>N</i> -acetyl-L-phenylalanine	2018-61-3	3.4.21.1
<i>N</i> -acetyl-L-phenylalanine ethyl ester	2361-96-8	3.4.21.1
<i>O</i> -acetyl-L-serine	66638-22-0	2.3.1.30
<i>N</i> -acetyl-L-tryptophan	1218-34-4	3.4.21.1
<i>N</i> -acetyl-L-tryptophan ethyl ester	2382-80-1	3.4.21.1
<i>N</i> -acetyl-L-tyrosine	537-55-3	3.4.21.1
<i>N</i> -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
allolactose	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
( <i>S</i> )-aminomethyl-dihydro- $\alpha$ -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
<i>N</i> -(benzyloxycarbonyl)-L-aspartic acid	1152-61-0	3.4.24.27
<i>N</i> -(benzyloxycarbonyl)-L-aspartyl-L-phenylalanine methyl ester		
	33605-72-0	3.4.24.27
( <i>Z</i> )=enolbutyryl-UDP- <i>N</i> -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 <sup>a</sup>	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
( <i>R</i> )-2-decanol	33758-15-5	3.1.1.3
( <i>R</i> )-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
( <i>S</i> )-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
( <i>R</i> )-2-dodecanol	99210-87-4	3.1.1.3
( <i>R</i> )-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-( <i>E</i> )-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- <i>O</i> - $\alpha$ -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- <i>O</i> - $\alpha$ -D-glucopyranosyl-D-fructofuranose	17606-72-3	3.2.1.3
3- <i>O</i> - $\alpha$ -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 <sup>a</sup>	Enzyme Commission Numbers
glutathionyl-ethyl-( <i>E</i> )-2-octenoate	214403-82-4	2.5.1.18
glutathionyl-methyl-( <i>E</i> )-2-octenoate	214403-83-5	2.5.1.18
glutathionyl-( <i>E</i> )-3-nonen-2-one	214403-84-6	2.5.1.18
glutathionyl-( <i>E</i> )-2-octenal	214403-85-7	2.5.1.18
4-(glutathionyl)-4-phenyl-2-butanone	104786-88-1	2.5.1.18
<b>D</b> -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
<i>N</i> -glycolyl- <b>D</b> -mannosamine	7483-19-4	4.1.3.3
<i>N</i> -glycolylneuramate	113-83-3	4.1.3.3
$\beta$ -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 <sub>2</sub> O	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 <sub>2</sub> O <sub>2</sub>	7722-84-1	1.1.3.4, 1.1.3.6, 1.11.1.6, 1.11.1.7
( <i>R</i> )-2-heptanol	6033-24-5	3.1.1.3
( <i>R</i> )-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- <i>exo</i> -hydroxycamphor	1607-84-7	1.14.15.1
6-hydroxycyclohex-1-ene-carboxyl-coenzyme A	148471-95-8	4.2.1.-
<b>D</b> -4-hydroxyphenylglycine	22818-40-2	3.5.1.11
4-hydroxyphenylpyruvate	156-39-8	1.3.1.12, 2.6.1.5
<b>L</b> -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
( <i>R</i> )-2-(4-isobutylphenyl)propionyl-coenzyme A	105567-78-0	5.1.2.-
( <i>S</i> )-2-(4-isobutylphenyl)propionyl-coenzyme A	135027-64-4	5.1.2.-
isochorismate	22642-82-6	5.4.99.6
$\alpha$ -isomaltose	499-40-1	3.2.1.3
$\beta$ -isomaltose	22352-61-0	3.2.1.3
( <i>S</i> )-lactate	79-33-4	1.1.1.27
lactose	63-42-3	3.2.1.23
lactulose	4618-18-2	3.2.1.23
<b>L</b> -leucine	61-90-5	2.6.1.42
$\alpha$ -lipoate	1077-28-7	1.4.4.2, 1.8.1.4
lyxose	1114-34-7	3.2.1.3
<b>D</b> -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 <sup>a</sup>	Enzyme Commission Numbers
1- <i>O</i> - $\alpha$ -D-mannopyranosyl-D-mannofuranose	197902-09-3	3.2.1.3
6- <i>O</i> - $\alpha$ -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
$\alpha$ -D-melibiose	585-99-9	3.2.1.3
$\beta$ -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-( <i>E</i> )-octenoate	2396-85-2	2.5.1.18
4-methyl-2-oxopentanoate	816-66-0	2.6.1.42
$\beta$ -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
$\beta$ -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
$\beta$ -nicotinamide-adenine dinucleotide phosphate (oxidized)	53-59-8	1.1.1.67, 1.6.4.2
$\beta$ -nicotinamide-adenine dinucleotide phosphate (reduced)	2646-71-1	1.1.1.67, 1.6.4.2
( <i>R</i> )-2-nonanol	628-99-9	3.1.1.3
( <i>E</i> )-3-nonen-2-one	14309-57-0	2.5.1.18
( <i>R</i> )-2-nonyl butyrate	117636-46-1	3.1.1.3
O <sub>2</sub>	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
( <i>E</i> )-2-octenal	2548-87-0	2.5.1.18
( <i>R</i> )-2-octanol	5978-70-1	3.1.1.3
( <i>R</i> )-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 <sub>2</sub>	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
( <i>E</i> )-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 <sup>ω</sup> -phospho-L-arginine	108321-86-4	2.7.3.3
( <i>Z</i> )-phosphoenolbutyrate	31302-64-4	2.5.1.7
<i>O</i> -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 <sup>a</sup>	Enzyme Commission Numbers
3-phospho-D-glyceroyl phosphate	38168-82-0	2.7.2.3
$\beta$ -phosphoguanidinopropionate	55601-59-7	2.7.3.2
<i>N</i> <sup>ω</sup> -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 <i>E</i> <sub>2</sub>	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
tributylglycerol	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-tryptophan	73-22-3	4.2.1.20
L-tyrosine	60-18-4	2.6.1.5
( <i>R</i> )-2-undecanol	85617-06-7	3.1.1.3
( <i>R</i> )-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- <i>N</i> -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

<sup>a</sup>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	$\beta$ -nicotinamide-adenine dinucleotide (oxidized)
ATP	adenosine 5'-triphosphate	NADH	$\beta$ -nicotinamide-adenine dinucleotide (reduced)
Bicine	<i>N,N</i> -bis(2-hydroxyethyl)glycine	NADP	$\beta$ -nicotinamide-adenine dinucleotide phosphate (oxidized)
Ches	2-(cyclohexylamino)ethanesulfonic acid	NADPH	$\beta$ -nicotinamide-adenine dinucleotide phosphate (reduced)
CoA	coenzyme A	Pipes	piperazine- <i>N,N'</i> -bis(2-ethanesulfonic acid)
GDP	guanosine 5'-diphosphate	Tes	<i>N</i> -tris(hydroxymethyl)methyl-2-aminoethanesulfonic acid
Hepes	<i>N</i> -(2-hydroxyethyl)piperazine- <i>N'</i> -ethanesulfonic acid	Tris	tris(hydroxymethyl)aminomethane
Mes	2-( <i>N</i> -morpholino)ethanesulfonic acid	UDP	uridine 5'-diphosphate

## 7. Glossary of Symbols

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

<sup>a</sup>When needed, a subscript  $c$ ,  $m$ , or  $x$  is added to these quantities to designate a concentration, molality, or mole fraction basis.

<sup>b</sup>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., Jourdan, G. W., Roseman, S., *J. Biol. Chem.* **237**, 2447 (1962).
- 62COM/ROS Comb, D. G., Roseman, S., *Methods Enzymol.* **5**, 391 (1962).
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