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**Critical Evaluation of  
STABILITY CONSTANTS FOR NUCLEOTIDE  
COMPLEXES WITH PROTONS AND  
METAL IONS  
and the Accompanying Enthalpy Changes†**

*Prepared for publication by*

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# Critical evaluation of stability constants for nucleotide complexes with protons and metal ions and the accompanying enthalpy changes

## CONTENTS

I.	Introduction .....	1017
II.	Method of Evaluation.....	1017
III.	Reported Values .....	1017
	A. Nucleotide Enthalpy Changes Reported.....	1018
	B. Nucleotide Protonation Constants Reported.....	1023
	C. Nucleotide Metal Ion Formation Constants Reported.....	1031
IV.	Discussion of Constants	
	A. Enthalpy Changes Accompanying Complexation.....	1057
	1. Protonation Enthalpy Changes.....	1057
	2. Alkali Metal Complex Enthalpy Changes.....	1058
	3. Alkaline Earth Metal Complex Enthalpy Changes.....	1058
	4. Transition Metal Complex Enthalpy Changes.....	1059
	5. Other Metal Complex Enthalpy Changes.....	1059
	B. Protonation Constants.....	1059
	C. Metal Ion Complexation Constants	
	1. Alkali Metal Constants.....	1061
	2. Alkaline Earth Metal Constants.....	1063
	3. Transition Metal Constants.....	1067
	4. Other Metal Constants.....	1072
V.	Recommended Values .....	1072
	A. Recommended Nucleotide Protonation and Complexation Enthalpy Changes.....	1073
	B. Recommended Nucleotide Protonation Constants .....	1074
	C. Recommended Nucleotide Metal Ion Complexation Constants.....	1076
VI.	Bibliography.....	1078

## ABBREVIATIONS USED IN THIS STUDY

ADP	= Adenosine 5'-diphosphate	HEPES	= 4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid
AMP-2	= Adenosine 2'-monophosphate	IDP	= Inosine 5'-diphosphate
AMP-3	= Adenosine 3'-monophosphate	Im	= Imidazole
AMP-5	= Adenosine 5'-monophosphate	IMP-5	= Inosine 5'-monophosphate
AMPD	= 2-Amino-2-methyl-1,3-propanediol	ITP	= Inosine 5'-triphosphate
AQP	= Adenosine 5'-tetraphosphate	M	= Mol/dm <sup>3</sup>
ATP	= Adenosine 5'-triphosphate	Me	= methyl
Bar.	= Barbiturate buffer	MES	= 2-Morpholinoethane-sulfonic acid
BIS-TRIS	= 2,2-Bis(hydroxymethyl)-2,2',2''-nitrilotriethanol	NEM	= N-Ethylmorpholine
Bu	= butyl	PIPES	= Piperazine- <i>N,N'</i> -bis-(ethanesulfonic acid)
Cac.	= Cacodylate buffer	Pr	= propyl
CDP	= Cytosine 5'-diphosphate	TAPS	= 3-[Tris(hydroxymethyl)methyl-amino]propanesulfonic acid
CMP-3	= Cytosine 3'-monophosphate	TEA	= 2,2',2''-Nitrilotriethanol
CMP-5	= Cytosine 5'-monophosphate	TMP-5	= Thymidine 5'-monophosphate
const.	= constant	TP	= Triphosphate
corr	= corrected	TRIS	= Tris(hydroxymethyl)aminomethane
CTP	= Cytosine 5'-triphosphate	TTP	= Thymidine 5'-triphosphate
DP	= Diphosphate	UDP	= Uridine 5'-diphosphate
Et	= ethyl	UMP-3	= Uridine 3'-monophosphate
GDP	= Guanosine 5'-diphosphate	UMP-5	= Uridine 5'-monophosphate
GMP-3	= Guanosine 3'-monophosphate	UTP	= Uridine 5'-triphosphate
GMP-5	= Guanosine 5'-monophosphate		
GTP	= Guanosine 5'-triphosphate		

## I. INTRODUCTION

The nucleotides are very important in biological systems because they are components of nucleic acids and are involved in many enzymatic reactions. The importance of adenosine-5'-triphosphate (ATP) in energy storage, utilization, and release and its participation in metabolism has led to numerous studies of its properties and functions. Biological reactions often require the presence of certain metal ions or are inhibited by them. Therefore an accurate knowledge of the protonation and metal ion binding constants of the nucleotides is essential for a thorough understanding of their reactions in biological systems.

Many determinations of these metal ion complexation constants have been reported, especially the binding of  $Mg^{2+}$  with ATP, but the results are often rather contradictory. Most previous compilations of these constants, such as those of Phillips, et. al. (66P) and of Izatt, et. al. (71I), are not critical but simply list the reported constants. The selections in "Critical Stability Constants", Volumes 2 (76S) and 5 (81M), do not involve many of the measurements reported in biological journals and specific reasons for the selections are not given. This study attempts to evaluate all reported proton and metal ion binding constants of the nucleotides in aqueous solution and to recommend a reasonable and internally consistent set of values for use in quantitative assessment of their chemical and biochemical reactions.

The nucleotides consist of a purine (adenine, guanine, hypoxanthine, or xanthine) bound at the 9-position or a pyrimidine (cytosine, thymine, or uracil) bound at the 1-position to a sugar (ribose or 2-deoxyribose with thymine) to form a nucleoside (adenosine, guanosine, inosine, xanthosine, cytidine, thymidine, or uridine) which is bound to a mono- or a polyphosphate, usually at the 5-position of the ribose.

## II. METHOD OF EVALUATION

Selection of the binding constants is most easily accomplished by comparing literature values which were measured under identical conditions of temperature and ionic strength. Several closely agreeing values from different research groups implies that the constant is well substantiated while differing values implies one or more serious experimental or computational errors or perhaps that other variables are affecting the results. Sometimes a careful reading of the paper will disclose an error or an unjustified assumption, but more often there are insufficient details to identify the reason for the variation. If no such reason is apparent, the value supported by the majority is accepted and variant values are assumed to involve some unidentified error. Sometimes comparisons to values for similar complexes presents a choice between disparate values or imparts support or mistrust to a single value.

A variety of temperatures and ionic strengths have been used for measurements and consequently it is necessary to adjust these to the same conditions for comparison. A majority of measurements have been made at 25°C and 0.10 M ionic strength and these conditions were selected as the comparison standard. The temperature adjustment was made with the enthalpy values recommended in this paper as indicated in 76S. The ionic strength adjustment was made by comparison to values at different ionic strength reported in the same paper or by trends in ionic strength differences with a change of ionic charges.

With papers that report values at two or more conditions, only the one with the least adjustment was converted to 25°C and 0.10 M ionic strength. The ionic strength for measurements made in buffer solutions without supporting electrolyte was calculated from the buffer molarity and the pH of the solution.

## III. REPORTED VALUES

The enthalpy changes, protonation constants, and metal ion formation constants found in the literature are listed in Tables 1, 2, and 3.

The order of arrangement is hydrogen ion, alkali metals, alkaline earth metals, transition metals, and miscellaneous metals. Within each group the order is tetraphosphates, triphosphates, diphosphates, and monophosphates. Within each phosphate group the order is adenosine, guanosine, inosine, cytosine, uridine, and thymidine. Under each ligand in Table 1, the order is by year of reference while in Tables 2 and 3, the order is by supporting electrolyte or buffer salt ( $Bu_3EtN^+$ ,  $Pr_4N^+$ ,  $Me_4N^+$ , corr, NEM.HCl, TEA.HCl, TRIS.HCl,  $K^+$ ,  $Na^+$ ), ionic strength (smallest to largest except for zero ionic strength at start of metal ligand complex), and year of reference.

Enthalpy values in Table 1, which were calculated by the temperature variation method, are enclosed in parenthesis to emphasize their reduced accuracy.

Values of protonation constants measured in  $Li^+$ ,  $Rb^+$ , and  $Cs^+$  background electrolytes (56S,86D) have not been included in Table 2.

Values extrapolated to zero ionic strength are indicated by  $\rightarrow 0$ , while those calculated to zero using a formula are indicated by 0 corr. An entry with a ? indicates the original paper is not clear on that subject while (?) indicates that something is obviously wrong with the reported value.

In some papers, the anion of the background electrolyte was not identified. The identity of the anion should be insignificant in its effect on the magnitude of the constant at lower ionic strengths except in the presence of cations which form strong complexes with them, such as  $Hg^{2+}$  with  $Cl^-$ , but would be important above perhaps 1.0 M ionic strength.

The final recommended values are listed in Tables 4, 5, and 6 with an estimate of the uncertainty for each value. Tentatively recommended values (T) are based on only one reported measurement or more than one from the same research group, while recommended values (R) are based on two or more independent measurements.

Table 1. Nucleotide Enthalpy Changes Reported (kJ/mol)

## Protonation Enthalpy Changes

Ligand Metal Ion	Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ H + L	$\Delta H$ H + HL	$\Delta H$ H + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>ATP</b>									
H <sup>+</sup>	T	25,38	0.15	NaCl	(+2.5)	(0.0)			51A
	C'	25	+0	Me <sub>4</sub> N <sup>+</sup>	+5.0	-15.5			62C
	C'	25	0.02-0.07 <sup>a</sup>	Me <sub>4</sub> N <sup>+</sup>	+5.0	-17.6			62C
	C'	25	0.10	Me <sub>4</sub> N <sup>+</sup>	+5.0	-18.8			62C
	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+7.1)				63P,65P
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-2.1)	(-17.2)			66T
	T	5,15,25,35,45	0.20	Me <sub>4</sub> NBr	(+10.9)				77R
	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+9.6)	(+6.3)	(+7.1)	H+H <sub>3</sub> L=(+7.1) H+H <sub>4</sub> L=(+7.9)	78G
	T	25,50	0.10	NaCl	(+10.0)	(-27.2)			79Mb
	T	50,60,70	0.10	NaCl	(+15.9)	(-9.6)			79Mb
	T	15,20,25,30	0 corr	NaClO <sub>4</sub>	(+8.7)	(-14)			80Tb
	C	25	0.10	Et <sub>4</sub> NBr	-0.8	-15.1			81C
	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(+3)	(-13)			86D
	C'	25	0.10	NaClO <sub>4</sub>	+5.08	-8.3			87Sa
<b>GTP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+7.5)				65P
	T	25,35,45	0.10	KNO <sub>3</sub>	(-13.0)	(-18.0)			73T
<b>ITP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+6.7)				65P
	T	25,35,45	0.10	KNO <sub>3</sub>	(-5.9)	(-9.6)			73T
<b>CTP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+7.5)				65P
	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.1)	(-17.2)	(-18.4)		83R
<b>UTP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+8.4)				65P
	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.1)	(-18.4)	(-18.4)		83R
<b>ADP</b>									
H <sup>+</sup>	T	25,38	0.15	NaCl	(+1.3)	(-3.8)			51A
	C'	25	+0	Me <sub>4</sub> N <sup>+</sup>	+5.4	-17.2			62C
	C'	25	0.01-0.06 <sup>a</sup>	Me <sub>4</sub> N <sup>+</sup>	+3.8	-18.4			62C
	C'	25	+0.10	Me <sub>4</sub> N <sup>+</sup>	+2.1	-19.7			62C
	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+5.9)				63P,65P
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-5.0)	(-20.1)			67T
	T	5,15,25,35,45	0.20	Me <sub>4</sub> NBr	(+7.9)				77R
	T	5,15,25,35	0.10	KNO <sub>3</sub>	(-13.8)				78D
	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+8.8)	(+3.8)	(+14.6)	H+H <sub>3</sub> L=(+4.6)	78G
	T	15,20,25,30	0 corr	NaClO <sub>4</sub>	(+2.3)	(-10)			80Tb
	C'	25	0.10	NaClO <sub>4</sub>	+2.35	-14.1			87Sa
<b>GDP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+6.3)				65P
	T	5,15,25,35	0.10	KNO <sub>3</sub>	(-10.9)				78D
<b>IDP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+5.4)				65P
<b>CDP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+5.4)				65P
	T	? ,25,?	0.10	KNO <sub>3</sub>		(-23.0)			73B
	T	5,15,25,35	0.10	KNO <sub>3</sub>	(-9.2)				78D
<b>UDP</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+4.6)				65P
	T	5,15,25,35	0.10	KNO <sub>3</sub>	(-10.9)				78D
<b>AMP-5</b>									
H <sup>+</sup>	T	25,38	0.15	NaCl	(+3.8)	(-3.8)			51A
	C'	25	+0	Me <sub>4</sub> N <sup>+</sup>	+7.5	-17.6			62C
	C'	25	0.01-0.06 <sup>a</sup>	Me <sub>4</sub> N <sup>+</sup>	+4.2	-16.7			62C
	C'	25	+0.10	Me <sub>4</sub> N <sup>+</sup>	0.0	-15.9			62C
	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+3.8)				63P,65P
	C'	25	+0	Na <sup>+</sup>				H+(H <sub>1</sub> L)=-45.6	66Ia
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-7.9)	(-20.5)			67T
	T	6,14,24,31,39	0.10	KNO <sub>3</sub>	(+4.6)	(-17.6)			74B
	T	5,15,25,35,45	0.20	Me <sub>4</sub> NBr	(+8.8)				77R
	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+6.3)	(+10.0)	(+3.8)		78G
	T	15,20,25,30	0 corr	NaClO <sub>4</sub>	(+1.5)	(-18)			80Tb
	C'	25	0.10	NaClO <sub>4</sub>	+3.34	-11.9			87Sa
	C	25	0.10	KNO <sub>3</sub>	+2.1	-18.0			88A
	C	25	+0	NaCl	+3.6	-15.0			88R

Table 1 (continued)

Ligand Metal Ion	Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ H + L	$\Delta H$ H + HL	$\Delta H$ H + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>AMP-3</b>									
H <sup>+</sup>	T	25,38	0.15	NaCl	(-7.5)	(-19.2)			51A
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-6.3)	(-19.2)			67T
<b>AMP-2</b>									
H <sup>+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-6.7)	(-19.7)			67T
<b>GMP-5</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+6.3)				65P
<b>IMP-5</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+5.9)				65P
<b>CMP-5</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+5.9)				65P
	T	10-80	0 corr	NaCl		(-15.1)			70W
<b>UMP-5</b>									
H <sup>+</sup>	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+4.6)				65P
	T	20,30,40,50	0.10	?				H+(H <sub>1</sub> L)=(-27.6)	67A

**Metal Ion Complexation Enthalpy Changes**

Ligand Metal Ion	Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ M + L	$\Delta H$ M + HL	$\Delta H$ M + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>ATP</b>									
Li <sup>+</sup>	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(-3)	(+4)		M+ML=(+14)	86D
Na <sup>+</sup>	C	25	0.10	Et <sub>4</sub> NBr	-0.8				81C
	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(-1)	(+5)			86D
K <sup>+</sup>	T	10-40	0.10	Me <sub>4</sub> NBr	(0.0)				66P + 66T,73B
	C	25	0.10	Et <sub>4</sub> NBr	+1.3				81C
	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(+4)	(+8)			86D
Rb <sup>+</sup>	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(+5)				86D
Cs <sup>+</sup>	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(+8)				86D
Et <sub>4</sub> N <sup>+</sup>	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(-2)	(-1)			86D
Mg <sup>2+</sup>	T	1,23,43	0.10	NaCl	(+17.2)				57N
	T	25,64	0.11	Bu <sub>3</sub> EtNBr	(+19.2)				59B
	T	10,25,37	+0	Pr <sub>4</sub> NBr	(+21.3)	(+9.2)			66P
	T	10,25,37	0.10	Pr <sub>4</sub> NBr	(+13.8)	(+7.9)			66P
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+10.9)	(+14.2)			66T
	T	0,12,25	0.10	KNO <sub>3</sub>	(+16.3)				66T
	T	12,25,40	0.10	KNO <sub>3</sub>		(+10.0)			66T
	C	30	0.20	Me <sub>4</sub> NCl	+18.70				69B
	T	10,20,30	0.12	NaCl	(+19.2)				71B
	T	3,17,26,30,39	0.20	Me <sub>4</sub> NBr	(+18.8)				73Sa
	C	37	0.20	Me <sub>4</sub> NCl	+18.3			M+ML= +7.2	82S
	C'	25	0.10	NaClO <sub>4</sub>	+18.08	+9.57			87Sa
Ca <sup>2+</sup>	T	1,23,43	0.10	NaCl	(+19.2)				57N
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-3.8)	(-1.3)			66T
	T	10,25,35,45	0.25	Pr <sub>4</sub> N <sup>+</sup>	(-8)	(-13)	(-16)	M+ML=(-6)	86D
	C'	25	0.10	NaClO <sub>4</sub>	+13.45	+7.96			87Sa
Sr <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-12.6)	(-6.7)			66T
Ba <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-16.3)	(-8.8)			66T
<b>GTP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+18.0				73S
	T	25,35,45	0.10	KNO <sub>3</sub>	(+3.8)				73T
Ca <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-6.7)				73T
<b>ITP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+18.8				73S
	T	25,35,45	0.10	KNO <sub>3</sub>	(+6.3)				73T
Ca <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-4.6)				73T
<b>CTP</b>									
Mg <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(+10.0)	(+11.7)			83R
Ca <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-12.1)	(-13.0)			83R
<b>UTP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+18.4				73S
	T	25,35,45	0.10	KNO <sub>3</sub>	(+17.2)				83R
Ca <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-17.2)				83R

Table 1 (continued)

Ligand Metal Ion	Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ M + L	$\Delta H$ M + HL	$\Delta H$ M + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>ADP</b>									
Mg <sup>2+</sup>	T	25,35,64	0.11	Bu <sub>3</sub> EtNBr	(+20.9)				59B
	T	10,25,37	0 corr	Pr <sub>4</sub> NBr	(+18.0)	(+3.8)			66P
	T	10,25,37	0.10	Pr <sub>4</sub> NBr	(+15.1)	(+4.2)			66P
	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+15.1)	(+16.3)			67T
	C	30	0.20	Me <sub>4</sub> NBr	+13.18				69B
	C'	25	0.10	NaClO <sub>4</sub>	+17.53	+7.66			87Sa
Ca <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-5.0)	(-2.5)			67T
	C'	25	0.10	NaClO <sub>4</sub>	+13.80	+6.27			87Sa
Sr <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-11.3)	(-5.0)			67T
Ba <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-12.1)	(-7.5)			67T
<b>GDP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+14.2				73S
<b>UDP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+13.4				73S
<b>AMP-5</b>									
Mg <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+14.2)				67T
	C	30	0.20	Me <sub>4</sub> NBr	+7.45				69B
	C'	25	0.10	NaClO <sub>4</sub>	+5.71				87Sa
Ca <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-2.5)				67T
	C'	25	0.10	NaClO <sub>4</sub>	+4.23				87Sa
Sr <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-5.9)				67T
Ba <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-8.4)				67T
<b>AMP-3</b>									
Mg <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+14.6)				67T
Ca <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-2.5)				67T
Sr <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-3.8)				67T
Ba <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-7.9)				67T
<b>AMP-2</b>									
Mg <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+14.6)				67T
Ca <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-2.5)				67T
Sr <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
Ba <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-8.4)				67T
<b>GMP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+7.1				73S
<b>UMP</b>									
Mg <sup>2+</sup>	C	30	0.20	Me <sub>4</sub> NBr	+7.5				73S
<b>ATP</b>									
Mn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-12.6)	(-9.6)			66T
	T	2,12,25,32,47	0.01	NEM-HCl	(-20.5)				70J
	T	26,41	0.10	NaCl	(-10.5)				70J
	T	1,5,10,15,25,35,43	0.20	Me <sub>4</sub> NBr	(+37.7)				77R
	C	6	0.20	Me <sub>4</sub> NBr	+13.4				77R
	C	15	0.20	Me <sub>4</sub> NBr	+15.5				77R
	C	30	0.20	Me <sub>4</sub> NBr	+19.2				77R
Co <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-9.2)	(-8.8)			66T
	T	5,15,25,30,36	0.20	Me <sub>4</sub> NBr	(+36.4)				78Ga
	C	25	0.20	Me <sub>4</sub> NBr	+18.8				78Ga
Ni <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-10.5)	(-10.0)			66T
Cu <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-18.0)	(-12.6)		ML-H = (-33.5), MOHL-H = (-50), 2MOHL = (-26.8)	66T
	C	25	0.10	K <sup>+</sup> corr	+3.3	-14.6		ML + L = -10.5, M + ML = +18.0	83A
Zn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-11.3)	(-10.0)			66T
	C	25	0.10	K <sup>+</sup> corr	+16.3	+4.6		ML + L = -11.3, M + ML = +12.6	83A
<b>GTP</b>									
Mn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-8.8)				73T
Co <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-6.7)				73T
Ni <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-7.9)				73T
Cu <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-18.8)				73T
Zn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-7.5)				73T
<b>ITP</b>									
Mn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-10.0)				73T
Co <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-5.0)				73T
Ni <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-8.4)				73T
Cu <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-25.1)				73T
Zn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-7.1)				73T

Table 1 (continued)

Ligand Metal Ion	Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ M + L	$\Delta H$ M + HL	$\Delta H$ M + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>CTP</b>									
Mn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-18.8)	(-20.9)			83R
Co <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.1)	(-18.4)			83R
Ni <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-16.3)	(-20.9)			83R
Cu <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.9)	(-18.0)			83R
Zn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-18.0)	(-14.6)			83R
<b>UTP</b>									
Mn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-27.6)				76T,83R
Co <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.1)				76T,83R
Ni <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.9)				76T,83R
Cu <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-20.9)				76T,83R
Zn <sup>2+</sup>	T	25,35,45	0.10	KNO <sub>3</sub>	(-19.2)				76T,83R
<b>ADP</b>									
Mn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-10.0)	(-7.9)			67T
	T	2,12,25,32,47	0.01	NEM.HCl	(+10.9)				70J
	T	26,41	0.10	NaCl	(+15.1)				70J
	T	15,25,35,43	0.20	Me <sub>4</sub> NBr	(+14.6)				77R
	C	6	0.20	Me <sub>4</sub> NBr	+7.45				77R
	C	15	0.20	Me <sub>4</sub> NBr	+11.09				77R
	C	30	0.20	Me <sub>4</sub> NBr	+14.73				77R
Co <sup>2+</sup>	T	12,25,40	0.10	KNO <sub>3</sub>	(-8.4)	(-7.9)			67T
	T	15,25,37	0.20	Me <sub>4</sub> NBr	(+11.7)				80M
Ni <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-7.9)	(-8.8)			67T
	T	15,25,37	0.20	Me <sub>4</sub> NBr	(+5.4)				79M
	C	25	0.20	Me <sub>4</sub> NBr	+6.3				79M
Cu <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-17.2)	(-11.3)		ML-H = (-37.7)	67T
								2MOHL = (-25.9)	
Zn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-8.4)	(-7.9)		ML-H = (-41.4)	67T
								2MOHL = (-21.3)	
<b>AMP-5</b>									
Mn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
	T	15,25,35,45	0.20	Me <sub>4</sub> NBr	(+4.2)				77R
	C	6	0.20	Me <sub>4</sub> NBr	+4.2				77R
	C	15	0.20	Me <sub>4</sub> NBr	+7.9				77R
	C	30	0.20	Me <sub>4</sub> NBr	+9.6				77R
Co <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+4.6)				67T
	T	15,25,37	0.20	Me <sub>4</sub> NBr	(-0.4)				80M
Ni <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
	T	6,14,24,31,39	0.10	KNO <sub>3</sub>	(-13.0)			ML+L = (-13.8)	74B
	T	15,25,37	0.20	Me <sub>4</sub> NBr	(-8.8)				79M
	C	25	0.20	Me <sub>4</sub> NBr	-10.5				79M
Cu <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-8.4)				67T
	C	25	0.10	KNO <sub>3</sub>	-25.9	+13.0			88A
Zn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-5.0)				67T
<b>AMP-3</b>									
Mn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-3.8)				67T
Co <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+2.5)				67T
Ni <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
Cu <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-7.1)				67T
Zn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.6)				67T
<b>AMP-2</b>									
Mn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
Co <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(+2.9)				67T
Ni <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-4.2)				67T
Cu <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-7.9)				67T
Zn <sup>2+</sup>	T	0,12,25,40	0.10	KNO <sub>3</sub>	(-5.0)				67T
<b>ATP</b>									
Y <sup>3+</sup>	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-14.7)	(-18.5)			87Sb
La <sup>3+</sup>	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-9.7)	(-15.2)			87Sb
Nd <sup>3+</sup>	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-16.7)	(-17.3)			87Sb
Eu <sup>3+</sup>	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+42.3)				78G
	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-16.6)	(-19.8)			87Sb
Dy <sup>3+</sup>	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-11.8)	(-14.3)			87Sb
Tm <sup>3+</sup>	T	9,17,25,32,41,50	0.10	NaClO <sub>4</sub>	(-12.3)	(-17.7)			87Sb
<b>ADP</b>									
Eu <sup>3+</sup>	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+40.2)				78G
	T	15,25,35	0.20	Me <sub>4</sub> NBr	(+21)				text

Table 1 (continued)

Ligand Metal Ion Method	Temperature (degrees C)	Ionic Strength	Background Electrolyte	$\Delta H$ M + L	$\Delta H$ M + HL	$\Delta H$ M + H <sub>2</sub> L	Other $\Delta H$	Ref.
<b>AMP-5</b>								
Y <sup>3+</sup>	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+23.4)	(-16.2)		87Sb
La <sup>3+</sup>	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+17.4)	(-16.2)		87Sb
Nd <sup>3+</sup>	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+20.9)	(-6.8)		87Sb
Eu <sup>3+</sup>	T	5,15,25,35	0.20	Me <sub>4</sub> NBr	(+0.8)			78G
	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+18.8)	(-14.2)		87Sb
Dy <sup>3+</sup>	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+20.4)	(-13.1)		87Sb
Tm <sup>3+</sup>	T	9,18,25,33,41,50	0.10	NaClO <sub>4</sub>	(+20.6)	(-12)		87Sb

Method: C = batch calorimetry, C' = titration calorimetry, T = temperature variation

<sup>a</sup> Average of values in the given range of ionic strength. ( ) inclose less accurate temperature variation results.



Table 2. Nucleotide Protonation Constants Reported

Ligand		T, °C.	Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Metal Ion	Method					H+L	25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1		
<b>AQP</b>													
H <sup>+</sup>	gl	25	0.20	Pr <sub>4</sub> NCl	con	7.27	7.42						56S
	gl	25	0.20	Et <sub>4</sub> NCl	con	7.23	7.38						56S
	gl	25	0.20	Me <sub>4</sub> NCl	con	7.06	7.21						56S
	gl	20	0.10	KCl	con	6.79	6.80	4.09	4.05				57S
	gl	25	0.20	KCl	con	6.58	6.73						56S
	gl	25	0.20	NaCl	con	6.46	6.61						56S
<b>ATP</b>													
H <sup>+</sup>	gl	10	→0	Pr <sub>4</sub> NBr	act	7.62							63P
	gl	25	→0	Pr <sub>4</sub> NBr	act	7.68							63P
	gl	37	→0	Pr <sub>4</sub> NBr	act	7.73							63P
	gl	10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	act	7.64		4.68					86D
	gl	25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	act	7.65		4.53					86D
	gl	35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	act	7.66		4.42					86D
	gl	45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	act	7.66		4.32					86D
	gl	25	0 corr	NaCl	act			4.57					51A/ 76K
	gl	25	0 corr	NaClO <sub>4</sub>	act	7.26		3.98					80Tb
	gl	25	→0	NaClO <sub>4</sub>	act				1.91				83S
	gl	10	0.04	Pr <sub>4</sub> N <sup>+</sup>	con	7.09		4.29					86D
	gl	25	0.04	Pr <sub>4</sub> N <sup>+</sup>	con	7.11		4.12					86D
	gl	35	0.04	Pr <sub>4</sub> N <sup>+</sup>	con	7.11		4.02					86D
	gl	45	0.04	Pr <sub>4</sub> N <sup>+</sup>	con	7.12		3.92					86D
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	7.10	6.99						63P
	gl	25	0.15	Pr <sub>4</sub> NBr	mix	7.07							63P
	gl	10	0.16	Pr <sub>4</sub> N <sup>+</sup>	con	6.90		4.13					86D
	gl	25	0.16	Pr <sub>4</sub> N <sup>+</sup>	con	6.91	6.96	3.99	4.03				86D
	gl	35	0.16	Pr <sub>4</sub> N <sup>+</sup>	con	6.92		3.90					86D
	gl	45	0.16	Pr <sub>4</sub> N <sup>+</sup>	con	6.94		3.79					86D
	gl	25	0.20	Pr <sub>4</sub> NCl	mix	6.95	6.91						56S
	gl	25	0.20	Pr <sub>4</sub> NBr	mix	7.05							63P
	gl	10	0.25	Pr <sub>4</sub> N <sup>+</sup>	con	6.87		4.11					86D
	gl	25	0.25	Pr <sub>4</sub> N <sup>+</sup>	con	6.90		3.97					86D
	gl	35	0.25	Pr <sub>4</sub> N <sup>+</sup>	con	6.91		3.89					86D
	gl	45	0.25	Pr <sub>4</sub> N <sup>+</sup>	con	6.93		3.80					86D
	gl	10	0.49	Pr <sub>4</sub> N <sup>+</sup>	con	6.88		4.16					86D
	gl	25	0.49	Pr <sub>4</sub> N <sup>+</sup>	con	6.95		4.03					86D, 88G
	gl	35	0.49	Pr <sub>4</sub> N <sup>+</sup>	con	7.00		3.95					86D
	gl	45	0.49	Pr <sub>4</sub> N <sup>+</sup>	con	7.05		3.88					86D
	gl	10	1.00	Pr <sub>4</sub> N <sup>+</sup>	con	6.92		4.19					86D
	gl	25	1.00	Pr <sub>4</sub> N <sup>+</sup>	con	7.11		4.18					86D
	gl	35	1.00	Pr <sub>4</sub> N <sup>+</sup>	con	7.24		4.17					86D
	gl	45	1.00	Pr <sub>4</sub> N <sup>+</sup>	con	7.37		4.17					86D
	gl	10	0.04	Et <sub>4</sub> N <sup>+</sup>	con	7.08		4.23					86D
	gl	25	0.04	Et <sub>4</sub> N <sup>+</sup>	con	7.09		4.09					86D
	gl	35	0.04	Et <sub>4</sub> N <sup>+</sup>	con	7.10		3.99					86D
	gl	45	0.04	Et <sub>4</sub> N <sup>+</sup>	con	7.11		3.89					86D
	gl	30	0.10	Et <sub>4</sub> NBr	con	6.97	6.97	3.93	3.98				64O
	gl	25	0.10	Et <sub>4</sub> NBr	con	7.10	7.10	4.05	4.05				81C
	gl	25	0.10	Et <sub>4</sub> NClO <sub>4</sub>	con	6.93	6.93	4.00	4.00				87Sa
	gl	25	0.15	Et <sub>4</sub> NBr	con	6.98							54M
	gl	10	0.16	Et <sub>4</sub> N <sup>+</sup>	con	6.86		4.03					86D
	gl	25	0.16	Et <sub>4</sub> N <sup>+</sup>	con	6.88	6.93	3.89	3.93				86D
	gl	35	0.16	Et <sub>4</sub> N <sup>+</sup>	con	6.90		3.79					86D
	gl	45	0.16	Et <sub>4</sub> N <sup>+</sup>	con	6.91		3.70					86D
	gl	25	0.20	Et <sub>4</sub> NBr	mix?	6.90	6.86						54M
	gl	25	0.20	Et <sub>4</sub> NBr	mix	6.91	6.87						56S
	gl	10	0.25	Et <sub>4</sub> N <sup>+</sup>	con	6.82		3.98					86D
	gl	25	0.25	Et <sub>4</sub> N <sup>+</sup>	con	6.85		3.84					86D
	gl	35	0.25	Et <sub>4</sub> N <sup>+</sup>	con	6.87		3.76					86D
	gl	45	0.25	Et <sub>4</sub> N <sup>+</sup>	con	6.90		3.66					86D
	gl	25	0.30	Et <sub>4</sub> NBr	con	6.85							54M
	gl	10	0.49	Et <sub>4</sub> N <sup>+</sup>	con	6.82		3.89					86D
	gl	25	0.49	Et <sub>4</sub> N <sup>+</sup>	con	6.88		3.78					86D
	gl	35	0.49	Et <sub>4</sub> N <sup>+</sup>	con	6.92		3.74					86D
	gl	45	0.49	Et <sub>4</sub> N <sup>+</sup>	con	6.96		3.62					86D
	gl	10	1.00	Et <sub>4</sub> N <sup>+</sup>	con	6.85		3.77					86D
	gl	25	1.00	Et <sub>4</sub> N <sup>+</sup>	con	7.00		3.67					86D

Table 2. (continued)

Ligand		Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr	Other equilibria	Ref.
Metal Ion								H+L	25°,0.1	H+HL	25°,0.1			
<u>ATP</u>														
<u>H<sup>+</sup></u>														
	gl			35	1.00	Et <sub>4</sub> N <sup>+</sup>	con	7.10		3.60				86D
	gl			45	1.00	Et <sub>4</sub> N <sup>+</sup>	con	7.20		3.53				86D
	gl			25	0.04	Me <sub>4</sub> N <sup>+</sup>	con	7.06		4.09				86D
	gl			30	0.10	Me <sub>4</sub> NBr	con	6.81	6.81	3.83	3.88			66Pa
	gl			25	0.16	Me <sub>4</sub> N <sup>+</sup>	con	6.80	6.85	3.92	3.96			86D
	gl			25	0.20	Me <sub>4</sub> NBr	mix	6.76	6.72					56S
	gl			30	0.20	Me <sub>4</sub> NBr	mix	6.96	6.90					73Sa
	gl			5	0.20	Me <sub>4</sub> NBr	mix	6.84						77R
	gl			15	0.20	Me <sub>4</sub> NBr	mix	6.91						77R
	gl			25	0.20	Me <sub>4</sub> NBr	mix	6.97	6.91					77R
	gl			35	0.20	Me <sub>4</sub> NBr	mix	7.03						77R
	gl			45	0.20	Me <sub>4</sub> NBr	mix	7.10						77R
	gl			5	0.20	Me <sub>4</sub> NBr	mix	6.84	4.89		4.70(?)		H+H <sub>3</sub> L=3.90, H+H <sub>4</sub> L=3.77	78G
	gl			15	0.20	Me <sub>4</sub> NBr	mix	6.90	4.93		4.11		H+H <sub>3</sub> L=3.95, H+H <sub>4</sub> L=3.82	78G
	gl			25	0.20	Me <sub>4</sub> NBr	mix	6.97	6.91	4.96	4.87	4.16	H+H <sub>3</sub> L=3.99, H+H <sub>4</sub> L=3.86	78G
	gl			35	0.20	Me <sub>4</sub> NBr	mix	7.01	5.01		4.20		H+H <sub>3</sub> L=4.02, H+H <sub>4</sub> L=3.92	78G
	gl			70	0.20	Me <sub>4</sub> NCl	mix	7.32	7.3	4.3	3.8			80R
	gl			25	0.25	Me <sub>4</sub> N <sup>+</sup>	con	6.75		3.88				86D
	gl			25	0.49	Me <sub>4</sub> N <sup>+</sup>	con	6.71		3.85				86D
	int			23	0.60	Me <sub>4</sub> NCl	mix	7.0	7.1					62A
	gl			25	1.00	Me <sub>4</sub> N <sup>+</sup>	con	6.74		3.79				86D
	gl			10	0.04	K <sup>+</sup>	con	6.81		4.26				86D
	gl			25	0.04	K <sup>+</sup>	con	6.82		4.10				86D
	gl			35	0.04	K <sup>+</sup>	con	6.82		4.10				86D
	gl			45	0.04	K <sup>+</sup>	con	6.82		4.91				86D
	gl			20	0.10	KCl	con	6.50	6.50	4.05	4.00			56M
	gl			25	0.10	KCl	mix	6.73	6.62	4.26	4.15			58Wa
	gl			22?	0.10	KCl	mix?	6.50	6.39	4.12	3.96			60B
	gl			20	0.10	KCl	mix?	6.50	6.39	3.95	3.79			62H
	gl			0	0.10	KNO <sub>3</sub>	con	6.56		4.29				66T
	gl			12	0.10	KNO <sub>3</sub>	con	6.54		4.14				66T
	gl			25	0.10	KNO <sub>3</sub>	con	6.53	6.53	4.06	4.06			62T, 66T
	gl			40	0.10	KNO <sub>3</sub>	con	6.52		3.87				66T
	gl			15	0.10	KNO <sub>3</sub>	con	6.57	6.56	4.18	4.09			72F
	gl			35	0.10	KNO <sub>3</sub>	con	6.80	6.81	4.12	4.21			72T
	gl			25	0.10	KNO <sub>3</sub>	mix	6.81	6.70	4.20	4.09			78D
	gl			35	0.10	KNO <sub>3</sub>	con	6.67	6.68	3.90	3.99			79Mc
	gl			25	0.10	KCl	mix	6.72	6.61	4.38	4.27			80D
	gl			25	0.10	KNO <sub>3</sub>	con	6.54	6.54					81C
	nmr			30	0.10	KNO <sub>3</sub>	mix	6.63	6.52					84P
	gl			25	0.10	KNO <sub>3</sub>	mix?	6.86	6.75	4.05	3.94			85M
	gl			25	0.10	KNO <sub>3</sub> ?	con?	6.63	6.63	4.09	4.09			86C
	gl			10	0.16	K <sup>+</sup>	con	6.38		4.10				86D
	gl			25	0.16	K <sup>+</sup>	con	6.39	6.44	3.95	3.99			86D
	gl			35	0.16	K <sup>+</sup>	con	6.39		3.85				86D
	gl			45	0.16	K <sup>+</sup>	con	6.40		3.75				86D
	gl			25	0.20	KCl	mix	6.48	6.44					56S
	gl			22	0.25	KNO <sub>3</sub>	mix	6.9	6.9	4.34	4.35			84G
	gl			10	0.25	K <sup>+</sup>	con	6.24		4.07				86D
	gl			25	0.25	K <sup>+</sup>	con	6.25		3.92				86D
	gl			35	0.25	K <sup>+</sup>	con	6.26		3.83				86D
	gl			45	0.25	K <sup>+</sup>	con	6.27		3.73				86D
	gl			10	0.49	K <sup>+</sup>	con	6.04		4.05				86D
	gl			25	0.49	K <sup>+</sup>	con	6.07		3.92				86D
	gl			35	0.49	K <sup>+</sup>	con	6.08		3.84				86D
	gl			45	0.49	K <sup>+</sup>	con	6.10		3.75				86D
	gl			25	1.00	KNO <sub>3</sub>	con	6.09		3.97				71R, 76R
	gl			10	1.00	K <sup>+</sup>	con	5.86		4.03				86D
	gl			25	1.00	K <sup>+</sup>	con	5.94		3.93				86D
	gl			35	1.00	K <sup>+</sup>	con	6.00		3.85				86D
	gl			45	1.00	K <sup>+</sup>	con	6.06		3.78				86D
	gl			10	0.04	Na <sup>+</sup>	con	6.73		4.26				86D

Table 2. (continued)

Ligand		Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.	
Type	H+L						25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1				
<b>ATP</b>															
<b>H<sup>+</sup></b>															
	gl			25	0.04	Na <sup>+</sup>	con	6.76		4.10				86D	
	gl			35	0.04	Na <sup>+</sup>	con	6.77		4.01				86D	
	gl			45	0.04	Na <sup>+</sup>	con	6.79		3.90				86D	
	?			20	0.05	NaClO <sub>4</sub>	mix	6.53	6.1	4.60	4.4	2.17	2.1	75K	
	sp			25	0.10	NaCl	mix	6.5	6.4	4.1	4.0			56B	
	gl			20	0.10	NaClO <sub>4</sub>	mix	6.47	6.36	4.10	3.95			64Sa	
	gl			25	0.10	NaClO <sub>4</sub>	mix	6.42	6.31					67S	
	gl			25	0.10	NaCl	mix	6.87	6.76	4.47	4.36	2.0	1.9	H+H <sub>3</sub> L=1.0, 0.9	
	gl			50	0.10	NaCl	mix	7.02		4.06				79Mb	
	gl			60	0.10	NaCl	mix	7.08		4.00				79Mb	
	gl			65	0.10	NaCl	mix	7.14		4.00				79Mb	
	gl			70	0.10	NaCl	mix	7.17		3.97				79Mb	
	gl			25	0.10	NaClO <sub>4</sub>	con	6.39	6.39		3.98			80Tb	
	gl			25	0.10	NaClO <sub>4</sub>	con	6.45	6.45					81C	
	gl			9	0.10	NaClO <sub>4</sub>	con	6.47		4.18				82Sa	
	gl			17	0.10	NaClO <sub>4</sub>	con	6.48		4.10				82Sa	
	gl			25	0.10	NaClO <sub>4</sub>	con	6.51	6.51	4.03				82Sa, 87Sa	
	gl			32	0.10	NaClO <sub>4</sub>	con	6.53		3.96				82Sa	
	gl			41	0.10	NaClO <sub>4</sub>	con	6.56		3.86				82Sa	
	gl			50	0.10	NaClO <sub>4</sub>	con	6.58		3.79				82Sa	
	gl			20	0.10	NaNO <sub>3</sub>	mix	6.51	6.40	4.12	3.96			83W	
	gl			25	0.10	NaClO <sub>4</sub>	mix	6.51	6.40	4.03	3.92			84Sa	
	gl			25	0.10	NaNO <sub>3</sub>	mix	6.49	6.38	4.01	3.90			85T	
	gl			25	0.10	NaNO <sub>3</sub>	mix	6.47	6.36	4.00	3.89			87S	
	gl			25	0.10	NaCl	con?	6.47	6.47	4.00	4.00	2.17	2.17	H+H <sub>3</sub> L=2.0, 2.0, H+(H <sub>1</sub> L)=11.78, H+(H <sub>2</sub> L)=15 [L]=0.25 mM	87Sc
	gl			25	0.10	NaNO <sub>3</sub>	mix	6.51	6.40	3.99	3.88			88T	
	gl			25	0.10	NaNO <sub>3</sub>	mix	6.60		4.24		1.7	1.6	[L]=30 mM	88T
	gl			25	0.12	NaCl	con	6.51	6.52	4.02	4.03			78R	
	gl			25	0.15	NaCl	mix	6.48	6.41	4.00	3.91			51A	
	gl			38	0.15	NaCl	mix	6.50		4.00				51A	
	gl			25	0.15	NaClO <sub>4</sub>	con?	6.42	6.46					71M	
	gl			25	0.15	NaCl	con	6.39	6.43	4.05	4.07			83J	
	gl			25	0.15	NaCl	con	6.24	6.28	3.70	3.72			87J	
	gl			25	0.15	NaClO <sub>4</sub>	con	6.24	6.28	4.00	4.02	1.77	1.8	88B	
	gl			10	0.16	Na <sup>+</sup>	con	6.27		4.10				86D	
	gl			25	0.16	Na <sup>+</sup>	con	6.31	6.36	3.94	3.98			86D	
	gl			35	0.16	Na <sup>+</sup>	con	6.33		3.85				86D	
	gl			45	0.16	Na <sup>+</sup>	con	6.35		3.75				86D	
	gl			25	0.20	NaCl	mix	6.41	6.37					56S	
	gl			10	0.25	Na <sup>+</sup>	con	6.12		4.07				86D	
	gl			25	0.25	Na <sup>+</sup>	con	6.16		3.92				86D	
	gl			35	0.25	Na <sup>+</sup>	con	6.19		3.83				86D	
	gl			45	0.25	Na <sup>+</sup>	con	6.21		3.74				86D	
	gl			25	0.34	NaCl	mix	6.34		4.24				79Mb	
	gl			10	0.49	Na <sup>+</sup>	con	5.91		4.05				86D	
	gl			25	0.49	Na <sup>+</sup>	con	5.96		3.93				86D	
	gl			35	0.49	Na <sup>+</sup>	con	6.00		3.84				86D	
	gl			45	0.49	Na <sup>+</sup>	con	6.03		3.76				86D	
	gl			25	0.50	NaClO <sub>4</sub>	con	5.89		3.97				80Tb	
	nmr			32	0.50	Na <sub>2</sub> L	con	5.63		4.62				85B	
	gl			25	0.61	NaCl	mix	6.10		4.02				79Mb	
	gl			25	0.86	NaCl	mix	6.04		3.95				79Mb	
	gl			25	1.00	NaClO <sub>4</sub>	con	5.70		3.95				80Tb	
	gl			10	1.00	Na <sup>+</sup>	con	5.72		4.03				86D	
	gl			25	1.00	Na <sup>+</sup>	con	5.82		3.94				86D	
	gl			35	1.00	Na <sup>+</sup>	con	5.89		3.88				86D	
	gl			45	1.00	Na <sup>+</sup>	con	5.97		3.81				86D	
	gl			25	1.00	NaNO <sub>3</sub>	mix	5.75		3.99				[L]=0.50 mM	
	gl			25	1.00	NaNO <sub>3</sub>	mix	5.87		4.10				[L]=200 mM	
	gl			25	1.12	NaCl	mix	5.87		3.91				79Mb	
	gl			25	2.00	NaClO <sub>4</sub>	con	5.57		3.91				80Tb	

Table 2. (continued)

<u>Ligand</u>		T, °C.	Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Metal Ion	Method					H+L	25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1		
<b>GTP</b>													
H <sup>+</sup>	gl	25	-0	Pr <sub>4</sub> NBr	act	7.65							65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	7.06	6.95						65P
	gl	25	0.10	KNO <sub>3</sub>	con	7.10	7.10	3.0	3.0				73T
	gl	35	0.10	KNO <sub>3</sub>	con	7.04		2.9					73T
	gl	45	0.10	KNO <sub>3</sub>	con	6.96		2.8					73T
	sp	25	0.10	NaCl	mix	6.5	6.4	3.3	3.2			H+(H <sub>-1</sub> L) = 9.3	56B
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.6	68S
	sp	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.5	68S
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.79	75S
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.45	6.34						77S
<b>ITP</b>													
H <sup>+</sup>	gl	25	-0	Pr <sub>4</sub> NBr	act	7.68							65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	7.12	7.01						65P
	gl	25	0.10	KNO <sub>3</sub>	con	6.92	6.92	2.2	2.2				73T
	gl	35	0.10	KNO <sub>3</sub>	con	6.97(?)		2.3(?)					73T
	gl	45	0.10	KNO <sub>3</sub>	con	6.86		2.1					73T
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.2	68S
	sp	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.0	68S
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.26	75S
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.45	6.34						77Sa, 77C
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.50	6.39						77S
<b>CTP</b>													
H <sup>+</sup>	gl	25	-0	Pr <sub>4</sub> NBr	act	7.65							65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	7.10	6.99						65P
	gl	15	0.10	KNO <sub>3</sub>	con	6.63	6.63	4.85	4.75				72F
	gl	25	0.10	KNO <sub>3</sub>	con	10.10	10.10(?)	4.32	4.32	2.71	2.71	83R	
	gl	35	0.10	KNO <sub>3</sub>	con	9.99	9.99(?)	4.22		2.62		75T,	
	gl	45	0.10	KNO <sub>3</sub>	con	9.88	9.88(?)	4.13		2.51		83R	83R
	gl	25	0.10	KCl	con?	6.46	6.46	4.15	4.15				84M
	sp	25	0.10	NaCl	mix	6.6	6.5	4.8	4.7				56B
<b>UTP</b>													
H <sup>+</sup>	gl	25	0.10	NaClO <sub>4</sub>	mix	6.51	6.40						77S
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.54	6.43	4.53	4.42				84Sa
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.55	6.44	4.55	4.44				87S
	gl	25	-0	Pr <sub>4</sub> NBr	act	7.58							65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	7.01	6.90						65P
	gl	25	0.10	KNO <sub>3</sub>	con	6.82	6.82	4.14	4.14	2.95	2.95		83R
	gl	35	0.10	KNO <sub>3</sub>	con	6.72		4.05		2.86			76T, 83R
	gl	45	0.10	KNO <sub>3</sub>	con	6.60		3.94		2.75			83R
	sp	25	0.10	NaCl	mix	6.6	6.5					H+(H <sub>-1</sub> L) = 9.5	56B
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.5	68S
	sp	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.6	68S
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.70	75S
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.45	6.34						77S, 78F
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.46	6.35	2.0	1.9				85T
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.45	6.34						87S
<b>TTP</b>													
H <sup>+</sup>	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.8	68S
	sp	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 10.1	68S
	gl	25	0.10	NaClO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.89	75S
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.50	6.39						77S
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.52	6.41	2.0	1.9				87S
<b>ADP</b>													
H <sup>+</sup>	gl	10	-0	Pr <sub>4</sub> NBr	act	7.15							63P
	gl	25	-0	Pr <sub>4</sub> NBr	act	7.20							63P
	gl	37	-0	Pr <sub>4</sub> NBr	act	7.24							63P
	gl	25	-0	Me <sub>4</sub> N <sup>+</sup>	act	7.00		4.20					62I
	gl	25	0 corr	NaCl	act			4.20					51A/ 76K
	gl	25	0 corr	NaClO <sub>4</sub>	act	6.71		3.27					80Tb
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.80	6.69						63P
	gl	25	0.15	Pr <sub>4</sub> NBr	mix	6.79							63P
	gl	25	0.20	Pr <sub>4</sub> NBr	mix	6.78							63P
	gl	25	0.20	Pr <sub>4</sub> NCl	mix	6.68	6.61						56S

Table 2. (continued)

Ligand		Metal	Ion Method	T, °C.	Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Metal	Ion							H+L	25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1		
<b>ADP</b>															
<b>H<sup>+</sup></b>															
	gl		30	0.10	Et <sub>4</sub> NBr	con	6.65	6.66							64O
	gl		25	0.20	Et <sub>4</sub> NBr	mix	6.68	6.61							56S
	gl		25	0.22	Et <sub>4</sub> NBr	con	6.65	6.70							54M
	gl		25	0.20	Me <sub>4</sub> NBr	mix	6.62	6.55							56S
	gl		5	0.20	Me <sub>4</sub> NBr	mix	6.54								77R
	gl		15	0.20	Me <sub>4</sub> NBr	mix	6.60								77R
	gl		25	0.20	Me <sub>4</sub> NBr	mix	6.65	6.54							77R
	gl		35	0.20	Me <sub>4</sub> NBr	mix	6.68								77R
	gl		45	0.20	Me <sub>4</sub> NBr	mix	6.74								77R
	gl		5	0.20	Me <sub>4</sub> NBr	mix	6.56		4.58		3.89		H+H <sub>3</sub> L=3.77		78G
	gl		15	0.20	Me <sub>4</sub> NBr	mix	6.62		4.60		3.96		H+H <sub>3</sub> L=3.80		78G
	gl		25	0.20	Me <sub>4</sub> NBr	mix	6.68	6.57	4.62	4.50	4.08	3.96	H+H <sub>3</sub> L=3.83, 3.71		78G
	gl		35	0.20	Me <sub>4</sub> NBr	mix	6.72		4.65		4.15		H+H <sub>3</sub> L=3.85		78G
	gl		20	0.10	KCl	con	6.35	6.34	3.99	3.94					56M
	gl		25	0.10	KCl	mix	6.61	6.50	4.21	4.10					58Wa
	gl		0	0.10	KNO <sub>3</sub>	con	6.51		4.20						67T
	gl		12	0.10	KNO <sub>3</sub>	con	6.48		4.09						67T
	gl		25	0.10	KNO <sub>3</sub>	con	6.44	6.44	3.93	3.93					62Ta,
															67T
	gl		40	0.10	KNO <sub>3</sub>	con	6.41		3.73						67T
	gl		15	0.10	KNO <sub>3</sub>	con	6.41	6.39	4.05	3.95					72F
	gl		5	0.10	KNO <sub>3</sub>	mix	6.98								78D
	gl		15	0.10	KNO <sub>3</sub>	mix	6.98								78D
	gl		25	0.10	KNO <sub>3</sub>	mix	6.90	6.79							78D
	gl		35	0.10	KNO <sub>3</sub>	mix	6.82								78D
	gl		25	0.10	KCl	mix	6.51	6.40	4.18	4.07					80D
	nmr		30	0.10	KNO <sub>3</sub>	mix	6.66	6.56							84P
	gl		25	0.20	KCl	mix	6.40	6.33							56S
	gl		22	0.25	KNO <sub>3</sub>	mix	6.72	6.66							84G
	?		20	0.05	NaClO <sub>4</sub>	mix	6.79	6.4	4.52	4.4					75K
	sp		25	0.10	NaCl	mix	6.3	6.2	3.9	3.8					56B
	gl		25	0.10	NaClO <sub>4</sub>	con	6.04	6.04	3.27	3.27					80Tb
	gl		25	0.10	NaClO <sub>4</sub>	con	6.41	6.41	3.95	3.95					87Sa
	gl		25	0.15	NaCl	mix	6.26	6.17	3.95	3.84					51A
	gl		38	0.15	NaCl	mix	6.27		3.92						51A
	gl		25	0.15	NaClO <sub>4</sub>	con	6.20	6.22							71M
	gl		25	0.15	NaCl	con	6.08	6.10	3.81	3.81					87J
	gl		25	0.20	NaCl	mix	6.36	6.29							56S
	gl		25	0.50	NaClO <sub>4</sub>	con	5.62		3.28						80Tb
	gl		25	1.00	NaClO <sub>4</sub>	con	5.43		3.29						80Tb
	gl		25	2.00	NaClO <sub>4</sub>	con	5.26		3.30						80Tb
<b>GDP</b>															
<b>H<sup>+</sup></b>															
	gl		25	+0	Pr <sub>4</sub> NBr	act	7.19								65P
	gl		25	0.10	Pr <sub>4</sub> NBr	mix	6.82	6.71							65P
	gl		5	0.10	KNO <sub>3</sub>	mix	7.03								78D
	gl		15	0.10	KNO <sub>3</sub>	mix	7.01								78D
	gl		25	0.10	KNO <sub>3</sub>	mix	6.95	6.84							78D
	gl		35	0.10	KNO <sub>3</sub>	mix	6.88								78D
	sp		25	0.10	NaCl	mix	6.3	6.2	2.9	2.8			H+(H <sub>1</sub> L)=9.6		56B
<b>IDP</b>															
<b>H<sup>+</sup></b>															
	gl		25	+0	Pr <sub>4</sub> NBr	act	7.18								65P
	gl		25	0.10	Pr <sub>4</sub> NBr	mix	6.80	6.69							65P
<b>CDP</b>															
<b>H<sup>+</sup></b>															
	gl		25	+0	Pr <sub>4</sub> NBr	act	7.18								65P
	gl		25	0.10	Pr <sub>4</sub> NBr	mix	6.79	6.68							65P
	gl		15	0.10	KNO <sub>3</sub>	con	6.38	6.40	4.56	4.44					72F
	gl		25	0.10	KNO <sub>3</sub>	con			4.46	4.46					73B
	gl		5	0.10	KNO <sub>3</sub>	mix	6.51								78D
	gl		15	0.10	KNO <sub>3</sub>	mix	6.50								78D
	gl		25	0.10	KNO <sub>3</sub>	mix	6.45	6.34							78D
	gl		35	0.10	KNO <sub>3</sub>	mix	6.39								78D
	gl		25	0.10	KCl	con	6.22	6.22	4.2	4.2					84M
	sp		25	0.10	NaCl	mix	6.4	6.3	4.6	4.5					56B

Table 2. (continued)

<u>Ligand</u>		Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Metal Ion	Method				T, °C.	H+L	25°, 0.1	H+HL	25°, 0.1	H+H <sub>2</sub> L		
<u>UDP</u>												
H <sup>+</sup>	gl	25	-0	Pr <sub>4</sub> NBr	act	7.16						65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.79	6.68					65P
	gl	5	0.10	KNO <sub>3</sub>	mix	6.72						78D
	gl	15	0.10	KNO <sub>3</sub>	mix	6.71						78D
	gl	25	0.10	KNO <sub>3</sub>	mix	6.65	6.54					78D
	gl	35	0.10	KNO <sub>3</sub>	mix	6.58						78D
	sp	25	0.10	NaCl	mix	6.5	6.4				H+(H <sub>-1</sub> L)=9.4	56B
<u>AMP-5</u>												
H <sup>+</sup>	gl	10	-0	Pr <sub>4</sub> NBr	act	6.64						63P
	gl	25	-0	Pr <sub>4</sub> NBr	act	6.67						63P
	gl	37	-0	Pr <sub>4</sub> NBr	act	6.70						63P
	gl	20	-0	?	act	6.37		3.81				88R
	gl	25	-0	?	act	6.54		3.79				88R
	gl	30	-0	?	act	6.68		3.78				88R
	cal	25	0 corr	Na <sup>+</sup>	act						H+(H <sub>-1</sub> L)=13.1	66Ia
	gl	25	0 corr	NaCl	act			3.97				51A/ 76K
	gl	25	0 corr	NaClO <sub>4</sub>	act	6.23		3.87				80Tb
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.47	6.36					63P
	gl	25	0.15	Pr <sub>4</sub> NBr	mix	6.48						63P
	gl	25	0.20	Pr <sub>4</sub> NBr	mix	6.47						63P
	gl	25	0.20	Pr <sub>4</sub> NCl	mix	6.45	6.34					56S
	gl	25	0.10	Et <sub>4</sub> NCl	con	6.46	6.46	3.86	3.86			87Sa
	gl	25	0.20	Et <sub>4</sub> NCl	mix	6.45	6.34					56S
	gl	25	0.10	Me <sub>4</sub> NBr	mix	6.40	6.29					61T
	gl	25	0.20	Me <sub>4</sub> NCl	mix	6.40	6.29					56S
	gl	5	0.20	Me <sub>4</sub> NBr	mix	6.28						77R
	gl	15	0.20	Me <sub>4</sub> NBr	mix	6.33						77R
	gl	25	0.20	Me <sub>4</sub> NBr	mix	6.39	6.28					77R
	gl	35	0.20	Me <sub>4</sub> NBr	mix	6.44						77R
	gl	45	0.20	Me <sub>4</sub> NBr	mix	6.48						77R
	gl	5	0.20	Me <sub>4</sub> NBr	mix	6.30		3.78		3.70		78G
	gl	15	0.20	Me <sub>4</sub> NBr	mix	6.34		3.84		3.72		78G
	gl	25	0.20	Me <sub>4</sub> NBr	mix	6.41	6.30	3.91	3.79	3.75	3.63	78G
	gl	35	0.20	Me <sub>4</sub> NBr	mix	6.45		4.03		3.81		78G
	gl	20	0.10	KCl	con	6.14	6.13	3.81	3.76			56M
	gl	25	0.10	KCl	mix	6.30	6.19					61T
	gl	0	0.10	KNO <sub>3</sub>	con	6.38		4.15				67T
	gl	12	0.10	KNO <sub>3</sub>	con	6.31		3.98				67T
	gl	25	0.10	KNO <sub>3</sub>	con	6.23	6.23	3.80	3.80			62Ta, 67T
	gl	40	0.10	KNO <sub>3</sub>	con	6.16		3.62				67T
	gl	15	0.10	KNO <sub>3</sub>	con	6.25	6.23	3.96	3.86			72F
	gl	5	0.10	KNO <sub>3</sub>	con	6.19		4.06				74B
	gl	15	0.10	KNO <sub>3</sub>	con	6.20		3.94				74B
	gl	25	0.10	KNO <sub>3</sub>	con	6.21	6.21	3.82	3.82			74B
	gl	30	0.10	KNO <sub>3</sub>	con	6.23		3.77				74B
	gl	40	0.10	KNO <sub>3</sub>	con	6.28		3.70				74B
	gl	25	0.10	KNO <sub>3</sub>	con	6.20	6.20	3.81	3.81			75B
	gl	25	0.10	KCl	con	6.13	6.13	3.63	3.63			80D
	gl	25	0.10	KNO <sub>3</sub>	mix	6.30	6.19	3.84	3.73			80O
	gl	25	0.10	KNO <sub>3</sub>	con	6.19	6.19	3.78	3.78			88A
	gl	25	0.20	KCl	mix	6.32	6.21					56S
	sp	20	0.025	Na <sub>2</sub> HPO <sub>4</sub>	con			3.70				63S
	?	20	0.05	NaClO <sub>4</sub>	mix	6.60	6.4	3.86	3.8			75K
	sp	25	0.10	NaCl	mix	6.1	6.0	3.7	3.6			56B
	gl	25	0.10	NaClO <sub>4</sub>	mix	6.14	6.03					64S
	sp	25	0.10	NaCl	con			3.84	3.84			76O
	gl	25	0.10	NaClO <sub>4</sub>	con	6.10	6.10	3.73	3.73			76Ta
	gl	25	0.10	NaClO <sub>4</sub>	con	5.93	5.93	3.87	3.87			80Tb
	gl	9	0.10	NaClO <sub>4</sub>	con	6.20		4.03				82Sa
	gl	17	0.10	NaClO <sub>4</sub>	con	6.22		3.98				82Sa
	gl	25	0.10	NaClO <sub>4</sub>	con	6.27		3.90				82Sa
	gl	25	0.10	NaClO <sub>4</sub>	con	6.29	6.29	3.93	3.93			87Sa
	gl	33	0.10	NaClO <sub>4</sub>	con	6.31		3.84				82Sa
	gl	41	0.10	NaClO <sub>4</sub>	con	6.34		3.78				82Sa
	gl	50	0.10	NaClO <sub>4</sub>	con	6.37		3.71				82Sa
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.22	6.11	3.84	3.73	0.4	0.3	87T

Table 2. (continued)

Ligand		Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Type	H+L						25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1			
<b>AMP-5</b>														
H <sup>+</sup>	gl	25	0.10	NaNO <sub>3</sub>	mix	6.21	6.10	3.84	3.73				88Sa	
	gl	25	0.15	NaCl	mix	6.05	5.95	3.74	3.63				51A	
	gl	38	0.15	NaCl	mix	6.08		3.71					51A	
	gl	25	0.15	NaCl	con	6.04	6.05	3.73	3.73				87J	
	gl	25	0.20	NaCl	mix	6.29	6.18						56S	
	gl	8	0.20	NaClO <sub>4</sub>	con	6.03	6.01	4.09	3.91				77P	
	gl	25	0.20	NaCl	mix	6.37	6.26	3.57	3.45				79T	
	gl	25	0.30	NaClO <sub>4</sub>	con	6.33	6.35	3.90	3.90				87H	
	gl	25	0.50	NaClO <sub>4</sub>	con	5.90		3.89					80Tb	
	gl	25	1.00	NaClO <sub>4</sub>	con	5.98		3.92					80Tb	
	gl	25	2.00	NaClO <sub>4</sub>	con	6.18		3.98					80Tb	
<b>AMP-3</b>														
H <sup>+</sup>	gl	25	0.10	KCl	mix	6.55	6.44	3.93	3.82				58Wa	
	gl	0	0.10	KNO <sub>3</sub>	con	5.93		3.95					67T	
	gl	12	0.10	KNO <sub>3</sub>	con	5.88		3.80					67T	
	gl	25	0.10	KNO <sub>3</sub>	con	5.83	5.83	3.65	3.65				62Ta, 67T	
	gl	40	0.10	KNO <sub>3</sub>	con	5.78		3.49					67T	
	gl	15	0.10	KNO <sub>3</sub>	con	5.79	5.76	3.74	3.64				80Ta	
	sp	25	0.10	NaCl	con			3.66	3.66				76O	
	gl	25	0.10	NaClO <sub>4</sub>	con	5.73	5.73	3.50	3.50				76Ta	
	gl	25	0.10	NaNO <sub>3</sub>	mix	5.77	5.66	3.68	3.57				87T	
	gl	25	0.10	NaNO <sub>3</sub>	mix	5.77	5.66	3.70	3.59				89M	
	gl	25	0.15	NaCl	mix	5.88	5.78	3.65	3.54				51A	
	gl	38	0.15	NaCl	mix	5.82		3.50					51A	
<b>AMP-2</b>														
H <sup>+</sup>	gl	0	0.10	KNO <sub>3</sub>	con	6.12		4.03					67T	
	gl	12	0.10	KNO <sub>3</sub>	con	6.07		3.88					67T	
	gl	25	0.10	KNO <sub>3</sub>	con	6.01	6.01	3.71	3.71				67T	
	gl	40	0.10	KNO <sub>3</sub>	con	5.95		3.54					67T	
	gl	15	0.10	KNO <sub>3</sub>	con	6.07	6.04	3.86	3.76				72F	
	gl	15	0.10	KNO <sub>3</sub>	con	6.02	5.99	3.74	3.64				80Ta	
	gl	25	0.10	NaNO <sub>3</sub>	mix	5.96	5.85	3.75	3.64				87T	
	gl	25	0.10	NaNO <sub>3</sub>	mix	5.95	5.84	3.74	3.63				89M	
<b>GMP-5</b>														
H <sup>+</sup>	gl	25	+0	Pr <sub>4</sub> NBr	act	6.66							65P	
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.50	6.39						65P	
	sp	20	0.15	KCl	mix							H+(H <sub>-1</sub> L) = 9.47	63S	
	sp	20	0.025	Na <sub>2</sub> HPO <sub>4</sub>	mix							H+(H <sub>-1</sub> L) = 9.53	63S	
	sp	25	0.10	NaCl	mix	6.1	6.0	2.4	2.3			H+(H <sub>-1</sub> L) = 9.4	56B	
	sp	25	0.10	NaCl	con			2.34	2.34				76O	
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.25	6.14	2.43	2.32				88Ma	
	gl	37	0.15	NaCl	con	6.19	6.21	2.35	2.48			H+(H <sub>-1</sub> L) = 9.17	83C	
	gl	25	0.20	NaCl	mix	6.37	6.26	2.27	2.16				79T	
<b>GMP-3</b>														
H <sup>+</sup>	sp	25	0.10	NaCl	con			2.15	2.15				76O	
<b>IMP-5</b>														
H <sup>+</sup>	gl	25	+0	Pr <sub>4</sub> NBr	act	6.66							65P	
	gl	25	0 corr	KCl	act	6.62							71Ma	
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.45	6.34						65P	
	gl	25	0.10	KCl	con	6.19	6.19						71Ma	
	gl	15	0.20	NaClO <sub>4</sub>	con	5.93	5.92					H+(H <sub>-1</sub> L) = 9.15	81N	
	gl	25	0.30	NaClO <sub>4</sub>	con	5.91	5.93					H+(H <sub>-1</sub> L) = 8.89	87H	
	gl	25	0.97	KCl	con	5.91							71Ma	
	gl	25	1.93	KCl	con	5.93							71Ma	
<b>CMP-5</b>														
H <sup>+</sup>	gl	25	+0	Pr <sub>4</sub> NBr	act	6.62							65P	
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.42	6.31						65P	
	sp	10	0 corr	NaCl	con				4.58				70W	
	sp	20	0 corr	NaCl	con			4.48					70W	
	sp	30	0 corr	NaCl	con			4.39					70W	
	sp	40	0 corr	NaCl	con			4.31					70W	
	sp	50	0 corr	NaCl	con			4.23					70W	
	sp	60	0 corr	NaCl	con			4.16					70W	
	sp	70	0 corr	NaCl	con			4.09					70W	
	sp	80	0 corr	NaCl	con			4.02					70W	
	gl	25	0.10	KCl	mix	6.35	6.24	4.35	4.24				58Wa	
	gl	15	0.10	KNO <sub>3</sub>	con	6.27	6.26	4.52	4.40				72F	

Table 2. (continued)

Ligand		T, °C.	Ionic Streng.	Backgr. Electr.	Type	Log K corr		Log K corr		Log K corr		Other equilibria	Ref.
Metal	Ion					H+L	25°,0.1	H+HL	25°,0.1	H+H <sub>2</sub> L	25°,0.1		
<b>CMP-5</b>													
H <sup>+</sup>	gl	25	0.10	KNO <sub>3</sub>	con	6.30	6.30	4.36	4.36				80O
	gl	25	0.10	KCl	con	6.31	6.31	3.75	3.75				84M
	gl	35	0.10	KNO <sub>3</sub>	con	6.30	6.29	4.27	4.39				85K
	sp	20	0.025	Na <sub>2</sub> HPO <sub>4</sub>	con			4.30					63S
	sp	25	0.10	NaCl	mix	6.3	6.2	4.5	4.4				56B
	sp	10	0.10	NaCl	con			4.52					70W
	sp	20	0.10	NaCl	con			4.42	4.37				70W
	sp	33	0.10	NaCl	con			4.25					70W
	sp	35	0.10	NaCl	con			4.24					70W
	sp	50	0.10	NaCl	con			4.11					70W
	sp	57	0.10	NaCl	con			4.00					70W
	sp	65	0.10	NaCl	con			3.98					70W
	sp	80	0.10	NaCl	con			3.91					70W
	sp	25	0.10	NaCl	con			4.33	4.33				76O
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.19	6.08	4.33	4.22				88M
	sp	10	0.20	NaCl	con			4.50					70W
	sp	20	0.20	NaCl	con			4.37					70W
	sp	30	0.20	NaCl	con			4.29					70W
	sp	40	0.20	NaCl	con			4.18					70W
	sp	50	0.20	NaCl	con			4.10					70W
	sp	60	0.20	NaCl	con			3.99					70W
	sp	70	0.20	NaCl	con			3.93					70W
	sp	80	0.20	NaCl	con			3.89					70W
	gl	25	0.20	NaCl	mix	6.69	6.58	4.47	4.36				79T
	sp	20	1.00	NaCl	con			4.21					63S
	sp	20	1.00	NaCl	con			4.36					70W
	sp	35	1.00	NaCl	con			4.20					70W
	sp	50	1.00	NaCl	con			4.07					70W
	sp	65	1.00	NaCl	con			3.95					70W
	sp	80	1.00	NaCl	con			3.90					70W
<b>CMP-3</b>													
H <sup>+</sup>	sp	25	0.10	NaCl	con			4.24	4.24				76O
<b>UMP-5</b>													
H <sup>+</sup>	gl	25	→0	Pr <sub>4</sub> NBr	act	6.63							65P
	gl	25	0.10	Pr <sub>4</sub> NBr	mix	6.45	6.34						65P
	sp	20	0.025	Na <sub>2</sub> HPO <sub>4</sub>	con						H+(H <sub>-1</sub> L) = 9.44		63S
	gl	20	0.015	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.71		67A
	gl	30	0.015	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.55		67A
	gl	40	0.015	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.38		67A
	gl	50	0.015	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.25		67A
	sp	25	0.10	NaCl	mix	6.4	6.3				H+(H <sub>-1</sub> L) = 9.5		56B
	gl	20	0.10	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.43		67A
	gl	30	0.10	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.28		67A
	gl	40	0.10	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.11		67A
	gl	50	0.10	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 8.95		67A
	gl	20	0.20	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.34		67A
	gl	30	0.20	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.18		67A
	gl	40	0.20	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.01		67A
	gl	50	0.20	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 8.85		67A
	gl	20	0.30	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.24		67A
	gl	30	0.30	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 9.07		67A
	gl	40	0.30	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 8.91		67A
	gl	50	0.30	Na <sup>+</sup> ?	con						H+(H <sub>-1</sub> L) = 8.76		67A
	sp	25	0.10	NaCl	con						H+(H <sub>-1</sub> L) = 9.43		76O
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.15	6.04						84S
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.15	6.04	0.7	0.6		H+(H <sub>-1</sub> L) = 9.45		88M
<b>UMP-3</b>													
H <sup>+</sup>	sp	25	0.10	NaCl	con						H+(H <sub>-1</sub> L) = 9.23		76O
<b>TMP-5</b>													
H <sup>+</sup>	gl	20	0.10	NaClO <sub>4</sub>	mix	6.57	6.45	1.45	1.3		H+(H <sub>-1</sub> L) = 10.3		68R
	gl	25	0.10	NaNO <sub>3</sub>	mix	6.36	6.25				H+(H <sub>-1</sub> L) = 9.90		88M
	gl	25	0.20	NaCl	mix	6.15	6.04						79T

Method: cal = calorimetric, gl = potentiometric with glass electrode, int = interferometer,  
 nmr = nuclear magnetic resonance, sp = spectrophotometric  
 Type of constant: act = activity, con = concentration, mix = mixed



Table 3. Nucleotide Metal Ion Formation Constants Reported

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.	
<u>AQP</u> Li <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	1.90						excess Li	56S	
	gl		25	0.20	Et <sub>4</sub> NCl	1.86						excess Li	56S	
	gl		25	0.20	Me <sub>4</sub> NCl	1.68	1.78					excess Li	56S	
Na <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	1.43						excess Na	56S	
	gl		25	0.20	Et <sub>4</sub> NCl	1.38						excess Na	56S	
	gl		25	0.20	Me <sub>4</sub> NCl	1.17	1.27					excess Na	56S	
K <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	1.29						excess K	56S	
	gl		25	0.20	Et <sub>4</sub> NCl	1.24						excess K	56S	
	gl		25	0.20	Me <sub>4</sub> NCl	1.00	1.10					excess K	56S	
<u>ATP</u> Li <sup>+</sup>	gl		10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.57		0.4				ML+M= 0.0	86D	
		gl	25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.53		0.44				excess Li	86D	
		gl	35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.49		0.45				ML+M= 0.1	86D	
		gl	45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.47		0.48				excess Li	86D	
		gl	10	0.04	Pr <sub>4</sub> N <sup>+</sup>	2.04		0.02				ML+M= 0.2	86D	
		gl	25	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.99		0.03				excess Li	86D	
		gl	35	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.95		0.05				ML+M= 0.3	86D	
		gl	45	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.93		0.07				excess Li	86D	
		gl	10	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.83		-0.14				ML+M= -0.28	86D	
		gl	25	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.79	1.84	-0.10				excess Li	86D	
		gl	35	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.77		-0.08				ML+M= -0.4	86D	
		gl	45	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.74		-0.06				excess Li	86D	
		gl	25	0.20	Pr <sub>4</sub> NCl	1.57						excess Li	56S	
		gl	10	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.80		-0.15				ML+M= -0.5	86D	
		gl	25	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.78		-0.11				excess Li	86D	
		gl	35	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.76		-0.08				ML+M= -0.43	86D	
		gl	45	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.75		-0.08				excess Li	86D	
		gl	10	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.82		-0.1				ML+M= -0.34	86D	
		gl	25	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.83		-0.05				excess Li	86D	
		gl	35	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.89		-0.02				ML+M= -0.3	86D	
		gl	45	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.85		0.0				excess Li	86D	
		gl	10	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.86		-0.1				ML+M= -0.31	86D	
		gl	25	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.99		0.09				excess Li	86D	
		gl	35	1.00	Pr <sub>4</sub> N <sup>+</sup>	2.09		0.21				ML+M= -0.2	86D	
		gl	45	1.00	Pr <sub>4</sub> N <sup>+</sup>	2.2		0.3				excess Li	86D	
		gl	25	0.20	Et <sub>4</sub> NCl	1.53						ML+M= 0.1	86D	
	Na <sup>+</sup>	gl		25	0.20	Me <sub>4</sub> NCl	1.35	1.42					excess Li	56S
		gl		25	0.05-0.12	LiCl	1.74	1.73					excess Li	65B
		ise		25	0 corr	Na <sub>2</sub> H <sub>2</sub> L	2.36	1.56					pH=9.2	70M
		gl		10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.08		0.2				excess Na	86D
		gl		25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.06		0.2				excess Na	86D
		gl		35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.04		0.2				excess Na	86D
gl			45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.03		0.3				excess Na	86D	
gl			10	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.54		-0.2				excess Na	86D	

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.			
ATP	Na <sup>+</sup>	gl	25	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.52		-0.20				excess Na	86D			
		gl	35	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.50		-0.2				excess Na	86D			
		gl	45	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.44		-0.2				excess Na	86D			
		gl	10	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.35		-0.4					excess Na	86D		
		gl	25	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.32	1.37	-0.33					excess Na	86D		
		gl	35	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.31		-0.31					excess Na	86D		
		gl	45	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.30		-0.3					excess Na	86D		
		gl	25	0.20	Pr <sub>4</sub> NCl	1.16							excess Na	56S		
		gl	10	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.32		-0.4					excess Na	86D		
		gl	25	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.31		-0.34					excess Na	86D		
		gl	35	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.30		-0.3					excess Na	86D		
		gl	45	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.30		-0.3					excess Na	86D		
		gl	10	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.32		-0.4					excess Na	86D		
		gl	25	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.36		-0.29					excess Na	86D		
		gl	35	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.38		-0.2					excess Na	86D		
		gl	45	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.41		-0.2					excess Na	86D		
		gl	10	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.4		-0.3					excess Na	86D		
		gl	25	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.52		-0.13					excess Na	86D		
		gl	35	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.64		0.0					excess Na	86D		
		gl	45	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.7		0.1					excess Na	86D		
		gl	25	0.10	Et <sub>4</sub> NCl	1.57	1.57								81C	
		gl	25	0.10	Et <sub>4</sub> NCl	1.29	1.29								87Sa	
		gl	25	0.20	Et <sub>4</sub> NCl	1.04								excess Na	56S	
		gl	25	0.22	Et <sub>4</sub> NBr	1.00	1.08							excess Na	54M	
		gl	25	0.30	Et <sub>4</sub> NBr	0.85								excess Na	54M	
		sp	30	0.10	NEM.HCl	1.18	1.18							pH=8.0, excess Na	64O	
		sp	25	0.10	Me <sub>4</sub> NCl	1.23	1.23							pH=8.5, excess Na	78A	
		gl	25	0.10	Me <sub>4</sub> NCl	1.10	1.10							excess Na, from H	text	
		gl	25	0.20	Me <sub>4</sub> NCl	0.80	0.87							excess Na	56S	
		gl	25	0.05-0.30	NaCl	1.23	1.29							excess Na	65B	
		K <sup>+</sup>	ise	gl	25	0 corr	K <sub>2</sub> H <sub>2</sub> L	2.34	1.54					pH=9.2	70M	
				gl	10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.94		0.2					excess K	86D
				gl	25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.95		0.2					excess K	86D
gl	35			0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.96		0.3					excess K	86D		
gl	45			0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.97		0.3					excess K	86D		
gl	10			0.04	Pr <sub>4</sub> N <sup>+</sup>	1.39		-0.2					excess K	86D		
gl	25			0.04	Pr <sub>4</sub> N <sup>+</sup>	1.41		-0.17					excess K	86D		
gl	35			0.04	Pr <sub>4</sub> N <sup>+</sup>	1.42		-0.1					excess K	86D		
gl	45			0.04	Pr <sub>4</sub> N <sup>+</sup>	1.43		-0.1					excess K	86D		
gl	10			0.16	Pr <sub>4</sub> N <sup>+</sup>	1.20		-0.36					excess K	86D		
gl	25			0.16	Pr <sub>4</sub> N <sup>+</sup>	1.21	1.26	-0.30					excess K	86D		
gl	35			0.16	Pr <sub>4</sub> N <sup>+</sup>	1.23		-0.26					excess K	86D		
gl	45			0.16	Pr <sub>4</sub> N <sup>+</sup>	1.24		-0.2					excess K	86D		
gl	25			0.20	Pr <sub>4</sub> NCl	1.06							excess K	56S		
gl	10			0.25	Pr <sub>4</sub> N <sup>+</sup>	1.17		-0.4					excess K	86D		
gl	25			0.25	Pr <sub>4</sub> N <sup>+</sup>	1.20		-0.32					excess K	86D		
gl	35			0.25	Pr <sub>4</sub> N <sup>+</sup>	1.22		-0.3					excess K	86D		
gl	45			0.25	Pr <sub>4</sub> N <sup>+</sup>	1.24		-0.2					excess K	86D		
gl	10			0.49	Pr <sub>4</sub> N <sup>+</sup>	1.18		-0.4					excess K	86D		
gl	25			0.49	Pr <sub>4</sub> N <sup>+</sup>	1.25		-0.26					excess K	86D		
gl	35			0.49	Pr <sub>4</sub> N <sup>+</sup>	1.30		-0.2					excess K	86D		
gl	45			0.49	Pr <sub>4</sub> N <sup>+</sup>	1.35		-0.1					excess K	86D		
gl	10			1.00	Pr <sub>4</sub> N <sup>+</sup>	1.22		-0.3					excess K	86D		
gl	25			1.00	Pr <sub>4</sub> N <sup>+</sup>	1.42		-0.11					excess K	86D		
gl	35			1.00	Pr <sub>4</sub> N <sup>+</sup>	1.55		0.0					excess K	86D		
gl	45			1.00	Pr <sub>4</sub> N <sup>+</sup>	1.70		0.1					excess K	86D		
gl	25			0.10	Et <sub>4</sub> NCl	1.42	1.42								81C	
gl	25			0.20	Et <sub>4</sub> NCl	0.93								excess K	56S	
gl	25			0.20	Et <sub>4</sub> NCl	0.99	1.06							excess K	54M	
gl	25			0.30	Et <sub>4</sub> NCl	0.83								excess K	54M	
sp	30			0.10	NEM.HCl	1.15	1.15							pH=8.0, excess K	64O	
kin	25			0.095	Me <sub>4</sub> NCl	1.19	1.19							pH=7.5, excess K	70B	
gl	25			0.10	Me <sub>4</sub> NCl	0.98	0.98							excess K, from H	text	
gl	25	0.20	Me <sub>4</sub> NCl	0.66	0.73							excess K	56S			
Rb <sup>+</sup>	gl	25	0.20-0.60	KCl	0.95	1.16						excess K	65B			
		10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.96		0.2					excess Rb	86D			
		25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.98		0.4					excess Rb	86D			
		35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.99		0.5					excess Rb	86D			

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.				
												Remarks					
ATP	Rb <sup>+</sup>	gl	45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.00						excess Rb	86D				
		gl	10	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.42						excess Rb	86D				
		gl	25	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.44						excess Rb	86D				
		gl	35	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.45							excess Rb	86D			
		gl	45	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.46							excess Rb	86D			
		gl	10	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.21							excess Rb	86D			
		gl	25	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.24	1.29						excess Rb	86D			
		gl	35	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.26							excess Rb	86D			
		gl	45	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.27							excess Rb	86D			
		gl	10	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.18							excess Rb	86D			
		gl	25	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.23							excess Rb	86D			
		gl	35	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.26							excess Rb	86D			
		gl	45	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.27							excess Rb	86D			
		gl	10	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.17							excess Rb	86D			
		gl	25	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.28							excess Rb	86D			
		gl	35	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.32							excess Rb	86D			
		gl	45	0.49	Pr <sub>4</sub> N <sup>+</sup>	1.35							excess Rb	86D			
		gl	10	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.25							excess Rb	86D			
		gl	25	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.44							excess Rb	86D			
		gl	35	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.56							excess Rb	86D			
		gl	45	1.00	Pr <sub>4</sub> N <sup>+</sup>	1.66							excess Rb	86D			
		Cs <sup>+</sup>	gl	25	0.20-0.60	RbCl	Pr <sub>4</sub> N <sup>+</sup>	0.90	1.11					excess Rb	65B		
				10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.89							excess Cs	86D		
				25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.94							excess Cs	86D		
				35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.97							excess Cs	86D		
				45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	2.00							excess Cs	86D		
				10	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.35							excess Cs	86D		
				25	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.40							excess Cs	86D		
				35	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.43							excess Cs	86D		
				45	0.04	Pr <sub>4</sub> N <sup>+</sup>	1.46							excess Cs	86D		
				10	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.15							excess Cs	86D		
				25	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.20	1.25						excess Cs	86D		
				35	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.24							excess Cs	86D		
				45	0.16	Pr <sub>4</sub> N <sup>+</sup>	1.28							excess Cs	86D		
				10	0.25	Pr <sub>4</sub> N <sup>+</sup>	1.12							excess Cs	86D		
25	0.25			Pr <sub>4</sub> N <sup>+</sup>	1.19							excess Cs	86D				
35	0.25			Pr <sub>4</sub> N <sup>+</sup>	1.23							excess Cs	86D				
45	0.25			Pr <sub>4</sub> N <sup>+</sup>	1.28							excess Cs	86D				
10	0.49			Pr <sub>4</sub> N <sup>+</sup>	1.15							excess Cs	86D				
25	0.49			Pr <sub>4</sub> N <sup>+</sup>	1.24							excess Cs	86D				
35	0.49			Pr <sub>4</sub> N <sup>+</sup>	1.31							excess Cs	86D				
45	0.49			Pr <sub>4</sub> N <sup>+</sup>	1.4							excess Cs	86D				
10	1.00			Pr <sub>4</sub> N <sup>+</sup>	1.2							excess Cs	86D				
25	1.00			Pr <sub>4</sub> N <sup>+</sup>	1.40							excess Cs	86D				
35	1.00			Pr <sub>4</sub> N <sup>+</sup>	1.56							excess Cs	86D				
45	1.00			Pr <sub>4</sub> N <sup>+</sup>	1.72							excess Cs	86D				
Me <sub>4</sub> N <sup>+</sup>	gl			25	0.20-0.60	CsCl	Pr <sub>4</sub> N <sup>+</sup>	0.85	1.06					excess Cs	65B		
				25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.2							excess Me <sub>4</sub> N	86D		
				25	0.04	Pr <sub>4</sub> N <sup>+</sup>	0.68							excess Me <sub>4</sub> N	86D		
				25	0.16	Pr <sub>4</sub> N <sup>+</sup>	0.48	0.53						excess Me <sub>4</sub> N	86D		
				25	0.25	Pr <sub>4</sub> N <sup>+</sup>	0.47							excess Me <sub>4</sub> N	86D		
				25	0.49	Pr <sub>4</sub> N <sup>+</sup>	0.52							excess Me <sub>4</sub> N	86D		
				25	1.00	Pr <sub>4</sub> N <sup>+</sup>	0.7							excess Me <sub>4</sub> N	86D		
				Et <sub>4</sub> N <sup>+</sup>	gl	10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.1							excess Et <sub>4</sub> N	86D
						25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.05							excess Et <sub>4</sub> N	86D
						35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.0							excess Et <sub>4</sub> N	86D
45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	1.0									excess Et <sub>4</sub> N	86D				
10	0.04	Pr <sub>4</sub> N <sup>+</sup>	0.54									excess Et <sub>4</sub> N	86D				
25	0.04	Pr <sub>4</sub> N <sup>+</sup>	0.51									excess Et <sub>4</sub> N	86D				
35	0.04	Pr <sub>4</sub> N <sup>+</sup>	0.48									excess Et <sub>4</sub> N	86D				
45	0.04	Pr <sub>4</sub> N <sup>+</sup>	0.5									excess Et <sub>4</sub> N	86D				
10	0.16	Pr <sub>4</sub> N <sup>+</sup>	0.34									excess Et <sub>4</sub> N	86D				
25	0.16	Pr <sub>4</sub> N <sup>+</sup>	0.31			0.36						excess Et <sub>4</sub> N	86D				
35	0.16	Pr <sub>4</sub> N <sup>+</sup>	0.30							excess Et <sub>4</sub> N	86D						
45	0.16	Pr <sub>4</sub> N <sup>+</sup>	0.3							excess Et <sub>4</sub> N	86D						
10	0.25	Pr <sub>4</sub> N <sup>+</sup>	0.31							excess Et <sub>4</sub> N	86D						
25	0.25	Pr <sub>4</sub> N <sup>+</sup>	0.30							excess Et <sub>4</sub> N	86D						
35	0.25	Pr <sub>4</sub> N <sup>+</sup>	0.28							excess Et <sub>4</sub> N	86D						

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
<b>ATP</b>													
Et <sub>4</sub> N <sup>+</sup>	gl		45	0.25	Pr <sub>4</sub> N <sup>+</sup>	0.3			0.2			excess Et <sub>4</sub> N	86D
	gl		10	0.49	Pr <sub>4</sub> N <sup>+</sup>	0.33			0.2			excess Et <sub>4</sub> N	86D
	gl		25	0.49	Pr <sub>4</sub> N <sup>+</sup>	0.35			0.20			excess Et <sub>4</sub> N	86D
	gl		35	0.49	Pr <sub>4</sub> N <sup>+</sup>	0.4			0.2			excess Et <sub>4</sub> N	86D
	gl		45	0.49	Pr <sub>4</sub> N <sup>+</sup>	0.4			0.2			excess Et <sub>4</sub> N	86D
	gl		10	1.00	Pr <sub>4</sub> N <sup>+</sup>	0.4			0.3			excess Et <sub>4</sub> N	86D
	gl		25	1.00	Pr <sub>4</sub> N <sup>+</sup>	0.51			0.4			excess Et <sub>4</sub> N	86D
	gl		35	1.00	Pr <sub>4</sub> N <sup>+</sup>	0.6			0.4			excess Et <sub>4</sub> N	86D
	gl		45	1.00	Pr <sub>4</sub> N <sup>+</sup>	0.7			0.6			excess Et <sub>4</sub> N	86D
<b>ADP</b>													
Li <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	1.15						excess Li	56S
	gl		25	0.20	Et <sub>4</sub> NCl	1.15						excess Li	56S
	gl		25	0.20	Me <sub>4</sub> NCl	1.06	1.10					excess Li	56S
Na <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	0.83						excess Na	56S
	gl		25	0.20	Et <sub>4</sub> NCl	0.73						excess Na	56S
	gl		25	0.22	Et <sub>4</sub> NBr	0.65	0.70					excess Na	54M
	gl		25	0.10	Me <sub>4</sub> NCl	0.92	0.92					excess Na, from H	text
	gl		25	0.20	Me <sub>4</sub> NCl	0.62	0.66					excess Na	56S
	sp		25	0.10	Me <sub>4</sub> NCl	0.6	0.6					pH=8.5, excess Na	78A
K <sup>+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	2.18	1.56					pH=9.1	74F
	gl		25	0.20	Pr <sub>4</sub> NCl	0.74						excess K	56S
	gl		25	0.20	Et <sub>4</sub> NCl	0.65						excess K	56S
	gl		25	0.22	Et <sub>4</sub> NBr	0.68	0.73					excess K	54M
	kin		25	0.095	Me <sub>4</sub> NCl	0.77	0.77					pH=7.5, excess K	70B
	gl		25	0.10	Me <sub>4</sub> NCl	0.77	0.77					excess K, from H	text
	gl		25	0.20	Me <sub>4</sub> NCl	0.53	0.57					excess K	56S
<b>AMP-5</b>													
Li <sup>+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	0.61						excess Li	56S
	gl		25	0.20	Et <sub>4</sub> NCl	0.61						excess Li	56S
	gl		25	0.20	Me <sub>4</sub> NCl	0.50	0.52					excess Li	56S
Na <sup>+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	1.9	1.5					pH=9.1	76K
	gl		25	0.20	Pr <sub>4</sub> NCl	0.46						excess Na	56S
	gl		25	0.20	Et <sub>4</sub> NCl	0.34						excess Na	56S
	gl		25	0.10	Me <sub>4</sub> NCl	0.53	0.53					excess Na, from H	text
	gl		25	0.20	Me <sub>4</sub> NCl	0.15	0.17					excess Na	56S
	ix		25	0.25	Me <sub>4</sub> NBr	0.45	0.48						61T
K <sup>+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	1.9	1.5					pH=9.1	76K
	gl		25	0.20	Pr <sub>4</sub> NCl	0.20(?)						excess K	56S
	gl		25	0.20	Et <sub>4</sub> NCl	0.26						excess K	56S
	kin		25	0.095	Me <sub>4</sub> NCl	0.63	0.63					pH=7.5, excess K	70B
	gl		25	0.10	Me <sub>4</sub> NCl	0.35	0.35					excess K, from H	text
	gl		25	0.20	Me <sub>4</sub> NCl	0.00	0.02					excess K	56S
<b>AQP</b>													
Mg <sup>2+</sup>	gl		20	0.10	KCl	4.22	4.29	2.7	2.7			large [M]/[L]?	57S
<b>ATP</b>													
Mg <sup>2+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	6.06	4.83					ML+M=2.61 pH~9.2 large NaL const. extr. to [Na <sup>+</sup> ]=0	74M
	ise		25	0 corr	Na <sup>+</sup> corr	5.87	4.59						text
	ix		23	0 corr	Na <sup>+</sup> corr	4.76						large [L]	57N
	ix		25	0 corr	Pr <sub>4</sub> NBr	5.83		3.6					66P
	sp		25	0 corr	Bu <sub>3</sub> EtNBr	5.70						pH=8.8	59B/ 63G
	sp		25	0 corr	Bu <sub>3</sub> EtNBr							ML+M=2.5 pH=8.8	59B/ 74M
	sp		30	0 corr	Et <sub>4</sub> NBr	6.11						pH=8.0	64O/ 74M
	sp		25	0.11	Bu <sub>3</sub> EtNBr	4.58	4.60					ML+M=1.8 pH=8.8	59B
	sp		64	0.11	Bu <sub>3</sub> EtNBr	4.99						pH=8.8	59B
	sp		25	0.22	Bu <sub>3</sub> EtNBr	4.35						pH=8.8	59B
	ix		5	0.07	Pr <sub>4</sub> NBr	4.46						pH=8.7	66P
	ix		25	0.07	Pr <sub>4</sub> NBr	4.60						pH=8.7	66P
	ix		45	0.07	Pr <sub>4</sub> NBr	4.78						pH=8.7	66P
	ix		65	0.07	Pr <sub>4</sub> NBr	4.96						pH=8.7	66P
	ix		5	0.10	Pr <sub>4</sub> NBr	4.45						pH=8.7	66P
	ix		25	0.10	Pr <sub>4</sub> NBr	4.63		2.7	2.7			pH=8.7	66P
	ix		25	0.10	Pr <sub>4</sub> NBr	4.56	4.56					average of 66P	text

Table 3. (continued)

Ligand		Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
ATP	Mg <sup>2+</sup>													
		ix	45	0.10	Pr <sub>4</sub> NBr	4.81							pH=8.7	66P
		ix	65	0.10	Pr <sub>4</sub> NBr	4.92							pH=8.7	66P
		ix	5	0.17	Pr <sub>4</sub> NBr	4.38							pH=8.7	66P
		ix	25	0.17	Pr <sub>4</sub> NBr	4.54							pH=8.7	66P
		ix	45	0.17	Pr <sub>4</sub> NBr	4.70							pH=8.7	66P
		ix	65	0.17	Pr <sub>4</sub> NBr	4.85							pH=8.7	66P
		gl	25	0.20	Pr <sub>4</sub> NBr	3.47	3.66	1.49	1.59				large [M]/[L]	56Sa
		lit	25	0.25	Pr <sub>4</sub> N <sup>+</sup>	4.54	4.71	2.00	2.13				ML+M=1.5, 1.6 lit/86D	61N
		gl	25	0.10	Et <sub>4</sub> NBr	4.43							pH~6.9, assume pH=pKa maximum of 61N	61N
		gl	25	0.10	Et <sub>4</sub> NBr	4.56	4.56						pH=7.0, 8.7	text
		ix	25	0.10	Et <sub>4</sub> NBr	4.35	4.35						TRIS buffer	61N
		gl	30	0.10	Et <sub>4</sub> NBr	4.88	4.82	2.7	2.7	1.3				64O
		sp	30	0.10	Et <sub>4</sub> NBr	4.94	4.94						NEM buffer	64O
		kin	25	0.095	Me <sub>4</sub> NCl	4.87	4.87						pH=8.0 pH=7.5, large MgCl <sub>2</sub> const.	70B
		sp	25	0.10	Me <sub>4</sub> NCl	4.85	4.85						TEA buffer	78A
		gl	25	0.20	Me <sub>4</sub> N <sup>+</sup>	3.45	3.64	1.15	1.25				pH=9.0 large [M]/[L]	56Sa
		?	25	0.20	Me <sub>4</sub> NBr	4.30	4.49						few details	58M/ 59B
		cal	30	0.20	Me <sub>4</sub> NCl	4.69	4.82						pH=8.5, large [L], TEA buffer	69B
		gl	3	0.20	Me <sub>4</sub> NBr	4.34							pH=8.0 assume [H] = [Mg]	73Sa
		gl	17	0.20	Me <sub>4</sub> NBr	4.53							pH=8.0, assume [H] = [Mg]	73Sa
		gl	26	0.20	Me <sub>4</sub> NBr	4.62	4.79						pH=8.0 assume [H] = [Mg]	73Sa
		gl	30	0.20	Me <sub>4</sub> NBr	4.66							pH=8.0 assume [H] = [Mg]	73Sa
		gl	39	0.20	Me <sub>4</sub> NBr	4.75							pH=8.0 assume [H] = [Mg]	73Sa
		gl	70	0.20	Me <sub>4</sub> NCl								ML+H=5.36 MHL+H=3.9	80R
		cal	37	0.20	Me <sub>4</sub> NCl	4.73	4.78						ML+M=1.69 pH=8.0 large [L]	82S
		sp	30	0.30	Me <sub>4</sub> NCl	4.6	4.9						ML+M=1.6 pH=8.5 few details	68N
		ix	23	0.12	Na <sup>+</sup> corr		3.61	3.67					pH=8.8, large [L]	70Na
		ix	23	0.20	Na <sup>+</sup> corr	3.59							pH=8.6, large [L]	57L
		gl	25	0.50	Na <sup>+</sup> corr	4.50	4.60	2.1	2.2	1.7	1.7		ML+M=1.03,1.08	88G
		sp	25	0.0006	TEA.HCl	5.74	4.65						pH=9.0, buffer	78A
		ise	25	0.001	TEA.HCl	5.26							pH=9.0, buffer	78A
		sp	25	0.002	TEA.HCl	5.22							pH=8.5, buffer	78A
		sp	25	0.004	TEA.HCl	4.63							pH=8.0, buffer	78A
		ise	25	0.005	TEA.HCl	5.21							pH=8.0, buffer	78A
		sp	25	0.007	TEA.HCl	4.30							pH=7.5, buffer	78A
		ise	25	0.009	TEA.HCl	4.90	4.56						pH=7.0, buffer	78A
		sp	25	0.03	TEA.HCl	4.78	4.47						pH=8.1, buffer	63W
		sp	30	0.04	TEA.HCl	4.89	4.60						pH=8.0, buffer	64O
		sp	25	0.04	TEA.HCl	4.49	4.26						pH=8.0, buffer	79Ma
		sp	30	0.02	NEM.HCl	4.89	4.39						pH=8.0, buffer	64O
		sp	20	0.05	NEM.HCl	4.76	4.38						pH=8.0, buffer	74E
		kin	20	0.003	TRIS.HCl	4.68	3.85						large [M]/[L], pH=8.5 buffer	73L
		int	23	0.03	TRIS.HCl	4.87	4.58						pH=9.0, buffer	62A
		sp	25	0.04	TRIS.HCl	4.72	4.49						ML+M=1.52 pH=7.5 buffer	81B
		sp	30	0.05	TRIS.HCl	4.30	4.18						pH=8.0, buffer	64O
		sp	25	0.05	TRIS.HCl	4.51	4.39						pH=8.2, buffer	63W
		ix	30	0.05	TRIS.HCl	4.24	4.12						pH=7.5, buffer	77N

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.	
ATP Mg <sup>2+</sup>	sp		37	0.06	TRIS.HCl	4.79						pH=8.4, buffer	70N	
	sp		37	0.10	TRIS.HCl	4.46	4.33					pH=8.4, buffer	70N	
	sp		37	0.15	TRIS.HCl	4.11						pH=8.4, buffer	70N	
	sp		37	0.24	TRIS.HCl	3.67						pH=8.4, buffer	70N	
	gl		20	0.10	KCl	4.00	4.06	2.0	2.0			large [M]/[L]	56M	
	gl		25	0.10	KCl	4.04	4.04	2.16	2.16			large [M]/[L]	58Wa	
	gl		20	0.10	KCl	3.84	3.90	2.09	2.12	1.58		large [M]/[L]	62H	
	gl		0	0.10	KNO <sub>3</sub>	3.97		1.95						66T
	gl		12	0.10	KNO <sub>3</sub>	4.10		2.16						66T
	gl		25	0.10	KNO <sub>3</sub>	4.22	4.22	2.24	2.24					62T, 66T
	gl		25	0.10	KNO <sub>3</sub>	3.99		1.89					large [M]/[L]	62T
	gl		40	0.10	KNO <sub>3</sub>	4.28		2.29						66T
	gl		15	0.10	KNO <sub>3</sub>	4.05	4.17	2.18	2.23					72F
	kin		15	0.10	KNO <sub>3</sub>								ML+M=1.77	72Fa
	gl		35	0.10	KNO <sub>3</sub>	4.50	4.38	2.77	2.71				HL 0.1 too large	79Mc
	?		?	0.10	K <sub>2</sub> PIPES	4.28	4.3						pH=6.95, T=? buffer	80V
	nmr		30	0.10	KNO <sub>3</sub>	4.7	4.6	2.8	2.8				large [L]	84P
	sp		25	0.11	KCl	4.26	4.28						pH=8.8?	59B
	ise		37	0.15	KCl	4.08	4.15						0.02 M NaCl	73Ba
	epr		37	0.15	KCl	4.42	4.38						pH=7.2 BIS-TRIS buffer	78Gb
	sp		25	0.15	KCl	3.99	4.16						pH=7.2 HEPES buffer	81W
	gl		22	0.25	KNO <sub>3</sub>	4.73	5.06						pH=7.1 HL const. too large	84G
	gl		25	1.00	KNO <sub>3</sub>	3.22								76R
	ix		23	0.10	NaCl	4.04	4.06						TRIS buffer	58W
	sp		25	0.10	NaCl	4.36	4.36						pH=8.2 pH=8.5,TEA buffer	78A
	gl		25	0.10	NaClO <sub>4</sub>	4.24	4.24							78M
	gl		25	0.10	NaClO <sub>4</sub>	4.37	4.37	1.94	1.94				MHL+HL=3.13?	86C
	gl		25	0.10	NaNO <sub>3</sub>	4.29	4.29	2.42	2.42					87S
	gl		25	0.10	NaClO <sub>4</sub>	4.03	4.03	2.12	2.12					87Sa
	kin		20	0.12	NaCl	3.65	3.81						pH=7.2,buffer	71B
	gl		25	0.12	NaCl	4.01	4.04						large [M]/[L]?	78R
	ix		?	0.12	NaCl	3.82							Im, T=?	84J
	ix		?	0.12	NaCl	3.95	4.0						pH~7.0, Sulfate TRIS, T=?	84J
	ix		?	0.12	NaCl	3.94							pH~8.2, Sulfate AMPD, T=?	84J
	ix		1	0.15	NaCl	3.06							pH~9.0, Sulfate pH=8.6, large [L]	57N
	ix		23	0.15	NaCl	3.34	3.46						pH=8.6, large [L]	57N
	ix		43	0.15	NaCl	3.50							pH=8.6, large [L]	57N
	ix		?	0.25	NaCl	3.82	4.1						pH=8.2, TRIS, T=?	85J
	ix		?	dilute	?	3.9							pH=?, few details	80K
	nmr		25	0.16	MgSO <sub>4</sub>								ML+M=1.52, large [L]	81B
Ca <sup>2+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	6.37	5.09					ML+M=3.04, 2.51, large NaL const. pH=9.1	72M	
	gl		25	0 corr	Pr <sub>4</sub> NCl			3.90				large [M]/[L]	56Sa/ 74F	
	ise		25	0 corr	Na <sup>+</sup> corr	6.56	5.28					ML+M=2.89, 2.36, ML+L=2.29, pH=9.1 large NaL const.	85O	
	gl		10	0 corr	Pr <sub>4</sub> N <sup>+</sup>	5.5		3.0		2.0		ML+M=1.4	86D	
	gl		25	0 corr	Pr <sub>4</sub> N <sup>+</sup>	5.26		2.6		1.6		ML+M=1.2	86D	
	gl		35	0 corr	Pr <sub>4</sub> N <sup>+</sup>	5.25		2.6		1.6		ML+M=1.3	86D	
	gl		45	0 corr	Pr <sub>4</sub> N <sup>+</sup>	5.38		2.7		1.9		ML+M=1.4	86D	
	sp		25	0.11	Bu <sub>3</sub> EtNBr	4.45	4.47					pH=9.0	59B	
	gl		10	0.04	Pr <sub>4</sub> N <sup>+</sup>	4.4		2.1		1.4		ML+M=0.9	86D	
	gl		25	0.04	Pr <sub>4</sub> N <sup>+</sup>	4.16		1.81		1.1		ML+M=0.7	86D	
	gl		35	0.04	Pr <sub>4</sub> N <sup>+</sup>	4.16		1.8		1.1		ML+M=0.7	86D	
	gl		45	0.04	Pr <sub>4</sub> N <sup>+</sup>	4.29		2.0		1.4		ML+M=0.8	86D	

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.
ATP Ca <sup>2+</sup>	gl		10	0.16	Pr <sub>4</sub> N <sup>+</sup>	4.0		1.8		1.3		ML+M=0.7	86D
	gl		25	0.16	Pr <sub>4</sub> N <sup>+</sup>	3.75	3.87	1.51	1.60	0.9	0.9	ML+M=0.53, 0.58	86D
	gl		35	0.16	Pr <sub>4</sub> N <sup>+</sup>	3.76		1.51		0.9		ML+M=0.5	86D
	gl		45	0.16	Pr <sub>4</sub> N <sup>+</sup>	3.90		1.7		1.2		ML+M=0.6	86D
	gl		25	0.20	Pr <sub>4</sub> NCl	3.29	3.48	1.61		1.71		large [M]/[L]	56Sa
	gl		10	0.25	Pr <sub>4</sub> N <sup>+</sup>	3.91		1.8		1.3		ML+M=0.6	86D
	gl		25	0.25	Pr <sub>4</sub> N <sup>+</sup>	3.70		1.47		0.9		ML+M=0.51	86D
	gl		35	0.25	Pr <sub>4</sub> N <sup>+</sup>	3.72		1.48		0.9		ML+M=0.5	86D
	gl		45	0.25	Pr <sub>4</sub> N <sup>+</sup>	3.87		1.7		1.2		ML+M=0.6	86D
	gl		10	0.49	Pr <sub>4</sub> N <sup>+</sup>	3.9		1.8		1.3		ML+M=0.7	86D
	gl		25	0.49	Pr <sub>4</sub> N <sup>+</sup>	3.77		1.5		0.9		ML+M=0.6	86D
	gl		35	0.49	Pr <sub>4</sub> N <sup>+</sup>	3.84		1.6		1.0		ML+M=0.6	86D
	gl		45	0.49	Pr <sub>4</sub> N <sup>+</sup>	4.03		1.8		1.3		ML+M=0.7	86D
	gl		10	1.00	Pr <sub>4</sub> N <sup>+</sup>	3.9		1.9		1.4		ML+M=0.8	86D
	gl		25	1.00	Pr <sub>4</sub> N <sup>+</sup>	4.02		1.8		1.1		ML+M=0.7	86D
	gl		35	1.00	Pr <sub>4</sub> N <sup>+</sup>	4.24		1.9		1.3		ML+M=0.9	86D
	gl		45	1.00	Pr <sub>4</sub> N <sup>+</sup>	4.6		2.2		1.6		ML+M=1.0	86D
	gl		25	0.10	Et <sub>4</sub> NCl	3.92						assume pH=KHL	61N
	gl		25	0.10	Et <sub>4</sub> NCl	3.96	3.96					maximum of 61N	text
	ix		25	0.10	Et <sub>4</sub> NCl	3.97	3.97					TRIS buffer pH=7.0	61N
	gl		30	0.10	Et <sub>4</sub> NCl	4.51	4.47						64O
	int		23	0.09	Me <sub>4</sub> NCl	3.89	3.89					TRIS buffer pH=8.0	62A
	int		23	0.10	Me <sub>4</sub> NCl			1.45	1.46			acetate buffer pH=5.0	62A
	gl		25	0.20	Me <sub>4</sub> NCl	3.09	3.28	1.08	1.18			large [M]/[L]	62A
	gl		70	0.20	Me <sub>4</sub> NCl							ML+H=5.6	80R
	sp		25	0.10	Na <sup>+</sup> corr	3.90	3.90					pH=7.0	61N
	ix		23	0.15	Na <sup>+</sup> corr	3.14	3.26					large [L]	57N
	gl		25	0.50	Na <sup>+</sup> corr	4.10	4.20	1.93	1.99	1.54	1.58	ML+M=0.82, 0.87	88G
	sp		30	0.02	NEM.HCl	4.49	4.01					pH=8.0, buffer	64O
	gl		20	0.10	KCl	3.60	3.65	1.8	1.8			large [M]/[L]	56M
	gl		0	0.10	KNO <sub>3</sub>	4.10		2.34					66T
	gl		12	0.10	KNO <sub>3</sub>	3.99		2.21					66T
	gl		25	0.10	KNO <sub>3</sub>	3.97	3.97	2.13	2.13				62T, 66T
	gl		25	0.10	KNO <sub>3</sub>	3.74		1.78				large [M]/[L]	62T
	gl		40	0.10	KNO <sub>3</sub>	3.94		2.13					66T
	gl		35	0.10	KNO <sub>3</sub>	3.91	3.81	2.16	2.12				79Mc
	ise		20	0.24	KCl	2.60	2.92					pH=7.3	79B
	gl		22	0.25	KNO <sub>3</sub>	3.4	3.7					large HL const.	84G
	ix		37	0.10	NaBar.	4.06	3.96					barbiturate buffer pH=7.4	53D
	ix		23	0.10	NaCl	3.77	3.79					TRIS buffer pH=8.2	58W
	sp		25	0.10	NaCl	3.60	3.60					pH=7.0	61N
	gl		25	0.10	NaClO <sub>4</sub>	3.88	3.88						78M
	gl		25	0.10	NaClO <sub>4</sub>	4.03	4.03	2.31	2.31			MHL+ML=2.0	86C
	gl		25	0.10	NaNO <sub>3</sub>	3.91	3.91	2.20	2.20				87S
	gl		25	0.10	NaClO <sub>4</sub>	3.70	3.70	2.04	2.04				87Sa
gl		25	0.12	NaCl	3.7	3.7					large [M]/[L]?	78R	
ix		1	0.15	NaCl	2.65						large [L]	57N	
ix		23	0.15	NaCl	2.87	2.99					large [L]	57N	
ix		43	0.15	NaCl	3.12						large [L]	57N	
ix		?	0.25	NaCl	3.35	3.7					sulfate, buffer pH=7.5	85J	
Sr <sup>2+</sup>	ix		?	dilute	?	3.5						pH=?, few details	80K
	gl		25	0.20	Pr <sub>4</sub> NCl	3.03	3.22	1.48	1.58			large [M]/[L]	56Sa
	gl		25	0.10	Et <sub>4</sub> NBr	3.60						assume H = KHL	61N
	gl		25	0.10	Et <sub>4</sub> NBr	3.64	3.64					maximum of 61N	text
	gl		0	0.10	KNO <sub>3</sub>	3.80		2.17					66T
	gl		12	0.10	KNO <sub>3</sub>	3.66		2.11					66T
	gl		25	0.10	KNO <sub>3</sub>	3.54	3.54	2.05	2.05				62T, 66T
	gl		40	0.10	KNO <sub>3</sub>	3.45		2.00					66T
	gl		25	0.10	NaClO <sub>4</sub>	3.66	3.66	2.36	2.36			MHL+HL=1.8	86C
	ix		25	0.15	NaCl	3.15	3.25					pH=7.4, few details	60O

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.
<u>ATP</u> Ba <sup>2+</sup>	gl		25	0.10	Et <sub>4</sub> NBr	3.37	3.37					assume H = KHL	61N
	gl		0	0.10	KNO <sub>3</sub>	3.58		2.02					66T
	gl		12	0.10	KNO <sub>3</sub>	3.42		1.92					66T
	gl		25	0.10	KNO <sub>3</sub>	3.29	3.29	1.85	1.85				62T, 66T
	gl		40	0.10	KNO <sub>3</sub>	3.12		1.75					66T
<u>GTP</u> Mg <sup>2+</sup>	cal		30	0.20	Me <sub>4</sub> NBr	3.93	4.06	2.23	2.31			ML-H = -9.41 pH = 8.5, TEA buffer assume [H] = [Mg]	73S
	gl		25	0.10	KNO <sub>3</sub>	4.98	4.98						73T
	gl		35	0.10	KNO <sub>3</sub>	5.20(?)							73T
	gl		45	0.10	KNO <sub>3</sub>	5.03							73T
	ix		23	0.10	NaCl	4.02	4.04					large [M]/[L], pH = 8.2, TRIS buffer	58W
	gl		25	0.10	NaClO <sub>4</sub>	4.13	4.13						77S
	gl		25	0.10	KNO <sub>3</sub>	4.92	4.92						73T
	gl		35	0.10	KNO <sub>3</sub>	5.01(?)							73T
	gl		45	0.10	KNO <sub>3</sub>	4.85							73T
	ix		23	0.10	NaCl	3.58	3.59					large [M]/[L] pH = 8.2, TRIS buffer	58W
<u>ITP</u> Mg <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	3.73	3.73						77S
	cal		30	0.20	Me <sub>4</sub> NBr	3.91	4.04	2.26	2.34			ML-H = -9.03 assume [H] = [Mg] TEA buffer pH = 8.2	73S
	sp		25	0.03	TEA.HCl	5.00	4.69					pH = 8.1	63W
	sp		25	0.05	TRIS.HCl	4.78	4.66					pH = 8.2	63W
	gl		25	0.10	KNO <sub>3</sub>	3.76	3.76						73T
	gl		35	0.10	KNO <sub>3</sub>	4.08(?)							73T
	gl		45	0.10	KNO <sub>3</sub>	3.84							73T
	ix		23	0.10	NaCl	4.04	4.06					large [M]/[L] pH = 8.2, TRIS buffer	58W
	gl		25	0.10	NaClO <sub>4</sub>	4.08	4.08						77S
	gl		25	0.10	KNO <sub>3</sub>	3.41	3.41						73T
<u>Ca<sup>2+</sup></u>	gl		35	0.10	KNO <sub>3</sub>	3.59(?)							73T
	gl		45	0.10	KNO <sub>3</sub>	3.37							73T
	ix		23	0.10	NaCl	3.76	3.77					large [M]/[L] pH = 8.2, TRIS buffer	58W
	gl		25	0.10	NaClO <sub>4</sub>	3.73	3.73						77S
	gl		15	0.10	KNO <sub>3</sub>	4.03	4.15	2.18	2.22				72F
	kin		15	0.10	KNO <sub>3</sub>							ML + M = 1.77	72Fa
	gl		25	0.10	KNO <sub>3</sub>	4.19	4.19	3.85	3.85				83R
	gl		35	0.10	KNO <sub>3</sub>	4.21		3.93					75T
	gl		45	0.10	KNO <sub>3</sub>	4.30		3.98					83R
	ix		23	0.10	NaCl	4.01	4.03					large [M]/[L], pH = 8.2, TRIS buffer	58W
<u>Ca<sup>2+</sup></u>	gl		25	0.10	NaClO <sub>4</sub>	4.08	4.08						77S
	gl		25	0.10	NaNO <sub>3</sub>	4.20	4.20	2.3	2.3				87S
	gl		25	0.10	KNO <sub>3</sub>	4.16	4.16	3.84	3.84				83R
	gl		35	0.10	KNO <sub>3</sub>	4.13		3.81					75T
	gl		45	0.10	KNO <sub>3</sub>	4.03		3.70					83R
	ix		23	0.10	NaCl	3.81	3.82					large [M]/[L] pH = 8.2, TRIS buffer	58W
	gl		25	0.10	NaClO <sub>4</sub>	3.72	3.72						77S
	gl		25	0.10	NaNO <sub>3</sub>	3.91	3.91	2.21	2.21				87S
	cal		30	0.20	Me <sub>4</sub> NBr	4.14	4.27	2.46	2.54			assume [H] = [Mg] ML-H = -9.31, TEA buffer, pH = 8.5	73S
	gl		25	0.10	KNO <sub>3</sub>	5.42	5.42						83R
gl		35	0.10	KNO <sub>3</sub>	5.53							76T	
gl		45	0.10	KNO <sub>3</sub>	5.61							83R	



Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.
<u>UTP</u>	Mg <sup>2+</sup>	ix	23	0.10	NaCl	4.02	4.04					large [M]/[L] pH=8.2, TRIS buffer	58W
		gl	25	0.10	NaClO <sub>4</sub>	4.00	4.00						77S
	Ca <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	4.27	4.27	2.72	2.72				87S
		gl	25	0.10	KNO <sub>3</sub>	5.20	5.20						83R
		gl	35	0.10	KNO <sub>3</sub>	5.12							76T
		gl	45	0.10	KNO <sub>3</sub>	5.01							83R
		ix	23	0.10	NaCl	3.71	3.72					large [M]/[L] pH=8.2, TRIS buffer	58W
		gl	25	0.10	NaClO <sub>4</sub>	3.66	3.66						77S
		gl	25	0.10	NaNO <sub>3</sub>	3.94	3.94	2.74	2.74				87S
<u>UTP</u>	Mg <sup>2+</sup>	gl	25	0.10	NaClO <sub>4</sub>	4.18	4.18						77S
		gl	25	0.10	NaNO <sub>3</sub>	4.23	4.23						87S
	Ca <sup>2+</sup>	gl	25	0.10	NaClO <sub>4</sub>	3.78	3.78						77S
		gl	25	0.10	NaNO <sub>3</sub>	3.85	3.85						87S
<u>ADP</u>	Mg <sup>2+</sup>	sp	25	0 corr	Bu <sub>3</sub> EtNBr	4.10							59B/ 63G
		sp	25	0 corr	Bu <sub>3</sub> EtNBr	4.14							59B/ 74F
		ix	25	0 corr	Pr <sub>4</sub> NBr	4.27		2.5				pH=8.7	66P
		ise	25	0 corr	Na <sup>+</sup> corr	4.65	3.78					pH=9.1, ML+M=1.7, large NaL const.	74F
		sp	30	0 corr	NEM.HCl	4.39						pH=8.0	64O/ 74F
		sp	25	0.11	Bu <sub>3</sub> EtNBr	3.34	3.36					pH=7.9	59B
		sp	35	0.11	Bu <sub>3</sub> EtNBr	3.48						pH=7.9	59B
		sp	64	0.11	Bu <sub>3</sub> EtNBr	3.84						pH=7.9	59B
		sp	25	0.22	Bu <sub>3</sub> EtNBr	3.23						pH=7.9	59B
		ix	5	0.04	Pr <sub>4</sub> NBr	3.48						pH=8.7	66P
		ix	25	0.04	Pr <sub>4</sub> NBr	3.65						pH=8.7	66P
		ix	45	0.04	Pr <sub>4</sub> NBr	3.83						pH=8.7	66P
		ix	65	0.04	Pr <sub>4</sub> NBr	4.00						pH=8.7	66P
		ix	25	0.10	Pr <sub>4</sub> NBr	3.50	3.50	2.0	2.0			pH=8.7	66P
		ix	5	0.11	Pr <sub>4</sub> NBr	3.24						pH=8.7	66P
		ix	25	0.11	Pr <sub>4</sub> NBr	3.44						pH=8.7	66P
		ix	45	0.11	Pr <sub>4</sub> NBr	3.60						pH=8.7	66P
		ix	65	0.11	Pr <sub>4</sub> NBr	3.76						pH=8.7	66P
		ix	5	0.18	Pr <sub>4</sub> NBr	3.14						pH=8.7	66P
		ix	25	0.18	Pr <sub>4</sub> NBr	3.33						pH=8.7	66P
		ix	45	0.18	Pr <sub>4</sub> NBr	3.46						pH=8.7	66P
		ix	65	0.18	Pr <sub>4</sub> NBr	3.64						pH=8.7	66P
		gl	25	0.20	Pr <sub>4</sub> NCl	3.00	3.14	1.45	1.50			large [M]/[L]	56Sa
		kin	25	0.095	Me <sub>4</sub> NCl	3.63	3.63					large MgCl <sub>2</sub> const.	70B
		sp	25	0.10	Me <sub>4</sub> NCl	3.90	3.95					pH=7.5, pH=8.5, TEA buffer	78A
		gl	25	0.20	Me <sub>4</sub> N <sup>+</sup>	3.09	3.28	1.08	1.18			large [M]/[L]	56Sa
		cal	30	0.20	Me <sub>4</sub> NCl	3.69	3.79					TEA buffer, large [L]	69B
		ix	23	0.10	Na <sup>+</sup> corr	3.04	3.06					pH=8.5, large [L]	57N
		sp	25	0.0006	TEA.HCl	4.61	3.88					pH=9.0, buffer	78A
		ise	25	0.001	TEA.HCl	4.00	3.31					pH=9.0, buffer	78A
		sp	25	0.002	TEA.HCl	4.19						pH=8.5, buffer	78A
		sp	25	0.004	TEA.HCl	3.72						pH=8.0, buffer	78A
		ise	25	0.004	TEA.HCl	3.90						pH=8.0, buffer	78A
		sp	25	0.007	TEA.HCl	3.34						pH=7.5, buffer	78A
		ise	25	0.009	TEA.HCl	3.60						pH=7.0, buffer	78A
		sp	25	0.03	TEA.HCl	3.78	3.47					pH=8.1, buffer	63W
		sp	30	0.02	NEM.HCl	3.61	3.34					pH=8.0, buffer	64O
		sp	20	0.05	NEM.HCl	3.71	3.52					pH=8.0, buffer	74E
		ix?	30?	0.01?	TRIS.HCl?	3.10		2.03				conditions uncertain	83Ca
		ix	30	0.01	TRIS.HCl	3.28	2.90					pH=7.5, buffer	82V
		sp	25	0.05	TRIS.HCl	3.54	3.42					pH=8.2, buffer	63W
		ix	30	0.05	TRIS.HCl	3.08	2.95					pH=7.5, buffer	77N
		sp	?	0.14	TRIS.HCl	3.30	3.4					pH=8.0, buffer, T=?	83G
		sp	?	0.14	TRIS.HCl	3.35						pH=7.4, buffer, T=?	83G

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.	
<u>ADP</u> Mg <sup>2+</sup>	gl		20	0.10	KCl	3.11	3.15	1.5	1.5			large [M]/[L]	56M	
	gl		25	0.10	KCl	3.23	3.23	1.58	1.58			large [M]/[L]	58Wa	
	gl		0	0.10	KNO <sub>3</sub>	2.94		1.39					67T	
	gl		12	0.10	KNO <sub>3</sub>	3.05		1.51					67T	
	gl		25	0.10	KNO <sub>3</sub>	3.17	3.17	1.64	1.64				62Ta	
													67T	
	gl		40	0.10	KNO <sub>3</sub>	3.30		1.78					67T	
	gl		15	0.10	KNO <sub>3</sub>	3.21	3.29	1.55	1.60				72F	
	kin		15	0.10	KNO <sub>3</sub>								ML + M = 1.0	72Fa
	nmr		30	0.10	KNO <sub>3</sub>	4.1	4.1	2.9	2.9				large [L]	84P
	epr		37	0.15	KCl	3.37	3.34						BIS-TRIS buffer pH = 7.2	78Gb
	gl		22	0.25	KNO <sub>3</sub>	2.53	2.60						large HL const.	84G
	ix		23	0.10	NaCl	3.15	3.17						large [M]/[L]	58W
													pH = 8.2, TRIS buffer pH = 8.5, TEA buffer	78A
	Ca <sup>2+</sup>	sp		25	0.10	NaCl	3.90	3.90						
gl			25	0.10	NaClO <sub>4</sub>	3.28	3.28	1.90	1.90					87Sa
ix			?	dilute	?	2.9							pH = ?, few details	80K
ise			25	0 corr	Na <sup>+</sup> corr	4.46	3.59						ML + M = 2.47, 2.24, pH = 9.1, large NaL const.	74F
sp			25	0 corr	Bu <sub>3</sub> EtNBr	3.70							pH = 8.8	59B/ 74F
gl			25	0 corr	Pr <sub>4</sub> NCl				2.70				large [M]/[L]	56Sa/ 74F
sp			30	0 corr	NEM.HCl	4.15							pH = 8.0	64O/ 74F
sp			25	0.11	Bu <sub>3</sub> EtNBr	2.89	2.91						pH = 8.8	59B
gl			25	0.20	Pr <sub>4</sub> NCl	2.81	2.91	1.52	1.57				large [M]/[L]	56Sa
int			23	0.09	Me <sub>4</sub> NCl	2.93	2.92						pH = 8.0, buffer	62A
int			23	0.10	Me <sub>4</sub> NCl			1.36	1.37				pH = 5.0, buffer	62A
gl			25	0.20	Me <sub>4</sub> NCl	2.65	2.84	1.20	1.30				large [M]/[L]	56Sa
ix			23	0.10	Na <sup>+</sup> corr	2.84	2.85						large [L]	57N
sp			30	0.02	NEM.HCl	3.34	3.08						pH = 8.0, buffer	64O
sp			?	0.14	TRIS.HCl	2.78	2.9						buffer, T = ? pH = 8.0	83G
gl		20	0.10	KCl	2.78	2.81						large [M]/[L]	56M	
gl		0	0.10	KNO <sub>3</sub>	2.91		1.61						67T	
gl		12	0.10	KNO <sub>3</sub>	2.88		1.60						67T	
gl		25	0.10	KNO <sub>3</sub>	2.86	2.86	1.58	1.58					62Ta	
													67T	
gl		40	0.10	KNO <sub>3</sub>	2.80	1.54							67T	
ise		20	0.20	KCl	2.60	2.77							HEPES buffer pH = 7.3	79B
gl		22	0.25	KNO <sub>3</sub>	2.2	2.4						large HL const.	84G	
ix		37	0.10	NaBar.	3.74	3.67						barbiturate buffer pH = 7.4	53D	
												large [M]/[L]	58W	
												pH = 8.2, TRIS buffer		
Sr <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	2.90	2.90	0.59	0.59					87Sa
	gl		25	0.20	Pr <sub>4</sub> NCl	2.50	2.60	1.34	1.39				large [M]/[L]	56Sa
	gl		0	0.10	KNO <sub>3</sub>	2.70		1.60						67T
	gl		12	0.10	KNO <sub>3</sub>	2.63		1.57						67T
	gl		25	0.10	KNO <sub>3</sub>	2.54	2.54	1.53	1.53					62Ta
													67T	
Ba <sup>2+</sup>	gl		40	0.10	KNO <sub>3</sub>	2.43		1.48						67T
	gl		0	0.10	KNO <sub>3</sub>	2.53		1.55						67T
	gl		12	0.10	KNO <sub>3</sub>	2.45		1.50						67T
	gl		25	0.10	KNO <sub>3</sub>	2.36	2.36	1.44	1.44					62Ta
														67T
													67T	
<u>GDP</u> Mg <sup>2+</sup>	gl		40	0.10	KNO <sub>3</sub>	2.25	1.37							67T
	cal		30	0.20	Me <sub>4</sub> NBr	3.4	3.5						assume [H] = [Mg]	73S
<u>CDP</u> Mg <sup>2+</sup>	gl		15	0.10	KNO <sub>3</sub>	3.22	3.30	1.60	1.62					72F
	kin		15	0.10	KNO <sub>3</sub>								ML + M = 1.0	72Fa

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.		
UDP	Mg <sup>2+</sup>	cal	30	0.20	Me <sub>4</sub> NBr	3.45	3.52					assume [H] = [Mg]	73S		
		ix	23	0.10	NaCl	3.17	3.19					large [M]/[L] pH=8.2, TRIS buffer	58W		
AMP-5	Mg <sup>2+</sup>	ise	25	0 corr	Na <sup>+</sup> corr	2.57	2.04					large NaL const. pH=9.1	76K		
		gl	25	0 corr	Pr <sub>4</sub> NCl	2.62						large [M]/[L]	56Sa/ 76K		
		gl	25	0 corr	KNO <sub>3</sub>	2.75							62Ta/ 76K		
		ix	23	0 corr	NaCl	2.73							large [M]/[L]	58W/ 76K	
		gl	25	0.20	Pr <sub>4</sub> NCl	1.69	1.74						large [M]/[L]	56Sa	
		gl	25	0.20	Me <sub>4</sub> NCl	1.53	1.58						large [M]/[L]	56Sa	
		cal	30	0.20	Me <sub>4</sub> NCl	1.81	1.84						TEA buffer, large [L] pH=8.5	69B	
		ix	23	0.10	Na <sup>+</sup> corr	2.0	2.0						large [L]	57N	
		ix	30	0.01	TRIS.HCl	2.20	1.97						pH=7.5, buffer	77N	
		gl	20	0.10	KCl	1.69	1.71						large [M]/[L]	56M	
		gl	25	0.10	KCl	2.14	2.14						large [M]/[L]	58Wa	
		gl	0	0.10	KNO <sub>3</sub>	1.75								67T	
		gl	12	0.10	KNO <sub>3</sub>	1.85								67T	
		gl	25	0.10	KNO <sub>3</sub>	1.97	1.97							62Ta 67T	
		gl	40	0.10	KNO <sub>3</sub>	2.09								67T	
		gl	15	0.10	KNO <sub>3</sub>	1.80	1.85							72F	
		ix	23	0.10	NaCl	1.95	1.96							large [M]/[L] pH=8.2, TRIS buffer	58W
		gl	25	0.10	NaClO <sub>4</sub>	1.63	1.63							large [M]/[L]	64S
		gl	25	0.10	NaClO <sub>4</sub>	2.10	2.10								87Sa
		gl	25	0.10	NaNO <sub>3</sub>	1.60	1.60							large [M]/[L]	88Sa
		gl	25	0.20	NaCl	1.83	1.88			0.04					79T
		ise	25	0 corr	Na <sup>+</sup> corr	2.59	2.06							large NaL const. pH=9.1	76K
		gl	25	0 corr	Pr <sub>4</sub> NCl	2.42								large [M]/[L]	56Sa/ 76K
		gl	25	0 corr	KNO <sub>3</sub>	2.68									62Ta/ 76K
		ix	23	0 corr	NaCl	2.59								large [M]/[L] pH=8.2	58W/ 76K
		gl	25	0.20	Pr <sub>4</sub> NCl	1.43	1.48							large [M]/[L]	56Sa
		gl	25	0.20	Me <sub>4</sub> NCl	1.40	1.45							large [M]/[L]	56Sa
gl	20	0.10	KCl	1.41	1.42							large [M]/[L]	56M		
gl	0	0.10	KNO <sub>3</sub>	1.88									67T		
gl	12	0.10	KNO <sub>3</sub>	1.87									67T		
gl	25	0.10	KNO <sub>3</sub>	1.85	1.85								62Ta 67T		
gl	40	0.10	KNO <sub>3</sub>	1.83									67T		
ix	23	0.10	NaCl	1.76	1.77							large [M]/[L], pH=8.2, TRIS buffer	58W		
gl	25	0.10	NaClO <sub>4</sub>	1.39	1.39							large [M]/[L]	64S		
gl	25	0.10	NaClO <sub>4</sub>	2.03	2.03								87Sa		
gl	25	0.10	NaNO <sub>3</sub>	1.46	1.46							large [M]/[L]	88Sa		
gl	25	0.20	Pr <sub>4</sub> NCl	1.32	1.37							large [M]/[L]	56Sa		
gl	0	0.10	KNO <sub>3</sub>	1.88									67T		
gl	12	0.10	KNO <sub>3</sub>	1.83									67T		
gl	25	0.10	KNO <sub>3</sub>	1.79	1.79								62Ta 67T		
gl	40	0.10	KNO <sub>3</sub>	1.74									67T		
gl	25	0.10	NaNO <sub>3</sub>	1.24	1.24							large [M]/[L]	88Sa		
ix	25	0.15	NaCl	1.5	1.5							pH=7.4, few details	60O		
gl	0	0.10	KNO <sub>3</sub>	1.85									67T		
gl	12	0.10	KNO <sub>3</sub>	1.80									67T		
gl	25	0.10	KNO <sub>3</sub>	1.73	1.73								62Ta 67T		
gl	40	0.10	KNO <sub>3</sub>	1.66									67T		
gl	25	0.10	NaClO <sub>4</sub>	1.14	1.14							large [M]/[L]	64S		
gl	25	0.10	NaNO <sub>3</sub>	1.17	1.17							large [M]/[L]	88Sa		

Table 3. (continued)

<u>Ligand</u>															
Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Remarks	Ref.		
<b>AMP-3</b>															
Mg <sup>2+</sup>	gl	25	0.10	KCl	1.73	1.73						large [M]/[L]	58Wa		
	gl	0	0.10	KNO <sub>3</sub>	1.68								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.78								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.89	1.89							62Ta		
Ca <sup>2+</sup>	gl	40	0.10	KNO <sub>3</sub>	2.01								67T		
	gl	25	0.10	NaNO <sub>3</sub>	1.49	1.49						large [M]/[L]	89M		
	gl	0	0.10	KNO <sub>3</sub>	1.86								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.84								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.80	1.80							62Ta		
Sr <sup>2+</sup>	gl	40	0.10	KNO <sub>3</sub>	1.78								67T		
	gl	25	0.10	NaNO <sub>3</sub>	1.36	1.36						large [M]/[L]	89M		
	gl	0	0.10	KNO <sub>3</sub>	1.81								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.75								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.71	1.71							62Ta		
Ba <sup>2+</sup>	gl	40	0.10	KNO <sub>3</sub>	1.68								67T		
	gl	25	0.10	NaNO <sub>3</sub>	1.15	1.15						large [M]/[L]	89M		
	ix	25	0.16	NaCl	1.4	1.4						pH=7.2	54S		
	gl	0	0.10	KNO <sub>3</sub>	1.81								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.75								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.69	1.69							62Ta		
Mg <sup>2+</sup>	gl	40	0.10	KNO <sub>3</sub>	1.62								67T		
	gl	25	0.10	NaNO <sub>3</sub>	1.08	1.08						large [M]/[L]	89M		
<b>AMP-2</b>															
Mg <sup>2+</sup>	gl	0	0.10	KNO <sub>3</sub>	1.71								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.82								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.93	1.93							67T		
	gl	40	0.10	KNO <sub>3</sub>	2.05								67T		
	gl	15	0.10	KNO <sub>3</sub>	1.75	1.80							72F		
Ca <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.53	1.53						large [M]/[L]	89M		
	gl	0	0.10	KNO <sub>3</sub>	1.87								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.85								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.83	1.83							67T		
	gl	40	0.10	KNO <sub>3</sub>	1.81								67T		
Sr <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.43	1.43						large [M]/[L]	89M		
	gl	0	0.10	KNO <sub>3</sub>	1.85								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.79								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.74	1.74							67T		
	gl	40	0.10	KNO <sub>3</sub>	1.71								67T		
Ba <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.20	1.20						large [M]/[L]	89M		
	gl	0	0.10	KNO <sub>3</sub>	1.82								67T		
	gl	12	0.10	KNO <sub>3</sub>	1.77								67T		
	gl	25	0.10	KNO <sub>3</sub>	1.71	1.71							67T		
	gl	40	0.10	KNO <sub>3</sub>	1.64								67T		
	gl	25	0.10	NaNO <sub>3</sub>	1.12	1.12						large [M]/[L]	89M		
<b>GMP-5</b>															
Mg <sup>2+</sup>	cal	30	0.20	Me <sub>4</sub> NBr	1.76	1.79						assume [H] = [Mg]	73S		
	gl	25	0.20	NaCl	1.81	1.86	-0.30						79T		
Ca <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.53	1.53						large [M]/[L]	88Ma		
<b>CMP-5</b>															
Mg <sup>2+</sup>	gl	15	0.10	KNO <sub>3</sub>	1.75	1.79							72F		
	gl	25	0.10	NaNO <sub>3</sub>	1.54	1.54						large [M]/[L]	88M		
Ca <sup>2+</sup>	gl	25	0.20	NaCl	1.81	1.86	-0.29						79T		
	gl	25	0.10	NaNO <sub>3</sub>	1.40	1.40						large [M]/[L]	88M		
Sr <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.17	1.17						large [M]/[L]	88M		
Ba <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.11	1.11						large [M]/[L]	88M		
<b>CMP-3</b>															
Sr <sup>2+</sup>	ix	25	0.16	NaCl	1.6	1.6						pH=7.2	54S		
<b>UMP-5</b>															
Mg <sup>2+</sup>	cal	30	0.20	Me <sub>4</sub> NBr	1.70	1.73						assume [H] = [Mg]	73S		
	ix	23	0.10	NaCl	2.25	2.26						large [M]/[L]	58W		
Ca <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.48	1.48						pH=8.2, TRIS buffer	84S		
	gl	25	0.10	NaNO <sub>3</sub>	1.56	1.56						large [M]/[L]	88M		
	gl	25	0.10	NaNO <sub>3</sub>	1.44	1.44						large [M]/[L]	88M		
	gl	25	0.10	NaNO <sub>3</sub>	1.44	1.44						large [M]/[L]	88M		

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.
<b>UMP-5</b>													
Sr <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.25	1.25					large [M]/[L]	88M
Ba <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.13	1.13					large [M]/[L]	88M
<b>TMP-5</b>													
Mg <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.55	1.55					large [M]/[L]	88M
	gl		25	0.20	NaCl	1.76	1.81	0.63					79T
Ca <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.40	1.40					large [M]/[L]	88M
Sr <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.19	1.19					large [M]/[L]	88M
Ba <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	1.11	1.11					large [M]/[L]	88M
<b>ATP</b>													
Mn <sup>2+</sup>	ise		25	0 corr	Na <sup>+</sup> corr	6.49	5.21	4.57	3.70			pH~7.2, ML+M=3 large NaL const.	74M
	gl		25	0.20	Pr <sub>4</sub> NCl	3.98	4.17	1.57	1.67			large [M]/[L]	56Sa
	gl		30	0.10	Me <sub>4</sub> NBr	5.19	5.15	2.62	2.59				66Pa
	gl		1	0.20	Me <sub>4</sub> NBr	5.44						assume [H] = [Mn] pH = 7.5	77R
	gl		5	0.20	Me <sub>4</sub> NBr	5.45						assume [H] = [Mn] pH = 7.5	77R
	gl		10	0.20	Me <sub>4</sub> NBr	5.48						assume [H] = [Mn] pH = 7.5	77R
	gl		15	0.20	Me <sub>4</sub> NBr	5.54						assume [H] = [Mn] pH = 7.5	77R
	gl		25	0.20	Me <sub>4</sub> NBr	5.71	5.90					assume [H] = [Mn] pH = 7.5	77R
	gl		35	0.20	Me <sub>4</sub> NBr	5.96						assume [H] = [Mn] pH = 7.5	77R
	gl		43	0.20	Me <sub>4</sub> NBr	6.18						assume [H] = [Mn] pH = 7.5	77R
	epr		2	0.0085	NEM.HCl	5.87						pH = 8.0, buffer	70J
	epr		12	0.0085	NEM.HCl	5.69						pH = 8.0, buffer	70J
	epr		25	0.0085	NEM.HCl	5.52	4.85					pH = 8.0, buffer	70J
	epr		32	0.0085	NEM.HCl	5.45						pH = 8.0, buffer	70J
	epr		47	0.0085	NEM.HCl	5.34						pH = 8.0, buffer	70J
	gl		22	0.10	KCl	4.78	4.80					ML-H = -10.4, sulfate, large [L]	61B
	gl		20	0.10	KCl	4.52	4.56	2.61	2.64	2.03	1.37	ML+M=1.37 large [M]/[L]	62H
	gl		0	0.10	KNO <sub>3</sub>	4.97	2.55						66T
	gl		12	0.10	KNO <sub>3</sub>	4.82	2.48						66T
	gl		25	0.10	KNO <sub>3</sub>	4.78	4.78	2.39	2.39				62T
	gl		25	0.10	KNO <sub>3</sub>	4.70	2.18					large [M]/[L]	66T
	gl		40	0.10	KNO <sub>3</sub>	4.63	2.30						66T
	gl		35	0.10	KNO <sub>3</sub>	5.25	5.17	3.11	3.05				79Mc
	gl		25	0.10	KCl	4.85	4.85	2.93	2.93				80Db
	epr		37	0.15	KCl	5.15	5.15					BIS-TRIS buffer pH = 7.2	78Gb
	gl		22	0.25	KNO <sub>3</sub>	4.55	4.87					large HL const.	84G
	ix		23	0.10	NaCl	4.75	4.77					large [M]/[L]	58W
	epr		28	0.10	NaCac.	4.49	4.45					pH = 8.2, TRIS buffer cacodylate buffer pH = 6.0	73V
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -10.7	75S
	gl		25	0.10	NaClO <sub>4</sub>	4.70	4.70						77Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.91	4.91						78M
	gl		25	0.10	NaClO <sub>4</sub>	5.32	5.32	3.20	3.20	2.77		MHL+HL=2.35 ML+M=2.11	86C
	gl		25	0.10	NaClO <sub>4</sub>	5.01	5.01	2.74	2.74				87S
	epr		25	0.11	NaCl	4.75	4.77					NEM buffer pH = 8.0	70J
	ix		26	0.11	NaCl	4.60	4.62					NEM buffer pH = 8.0	70J
	ix		41	0.11	NaCl	4.52						NEM buffer pH = 8.0	70J
	gl		25	0.12	NaCl	4.56	4.60					large [M]/[L]?	78R
	gl		25	0.15	NaCl	4.72	4.82	2.80	2.85	2.29			83J
	ix		?	0.25	NaCl	4.13	4.4					buffer, sulfate, T = ? pH = 7.5	85J
	ix		?	dilute	?	4.23						pH = ?, few details	80K

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
ATP													
Fe <sup>2+</sup>		gl	25	1.00	KNO <sub>3</sub>	4.11		2.20					71R
		gl	25	0.12	NaCl	5.1	5.1						78R
Co <sup>2+</sup>		gl	30	0.10	Me <sub>4</sub> NBr	5.21	5.17	2.65	2.63				66Pa
		gl	5	0.20	Me <sub>4</sub> NBr	5.59						assume [H] = [Co] pH=7.1	78Ga
		gl	15	0.20	Me <sub>4</sub> NBr	5.74						assume [H] = [Co] pH=7.1	78Ga
		gl	26	0.20	Me <sub>4</sub> NBr	5.92	6.12					assume [H] = [Co] pH=7.1	78Ga
		gl	30	0.20	Me <sub>4</sub> NBr	6.10						assume [H] = [Co] pH=7.1	78Ga
		gl	36	0.20	Me <sub>4</sub> NBr	6.25						assume [H] = [Co] pH=7.1	78Ga
		gl	22?	0.10	KCl	4.53	4.57					sulfate, large [L]	60B
		gl	22	0.10	KCl	4.71	4.73					ML-H = 9.4, sulfate large [L]	61B
		kin	25	0.10	KNO <sub>3</sub>	4.66	4.66						64H
		gl	0	0.10	KNO <sub>3</sub>	4.80		2.45					66T
		gl	12	0.10	KNO <sub>3</sub>	4.69		2.39					66T
		gl	25	0.10	KNO <sub>3</sub>	4.66	4.66	2.32	2.32				62T
		gl	25	0.10	KNO <sub>3</sub>	4.58		2.14					66T
		gl	40	0.10	KNO <sub>3</sub>	4.55		2.24				large [M]/[L]	62T
		gl	25	0.10	KCl	4.36	4.36	2.73	2.73				66T
		ix	20	0.05	NaClO <sub>4</sub>	6.80	6.72						80Da
		ix	23	0.10	NaCl	4.62	4.64					large [L] large [M]/[L] pH=8.2, TRIS buffer	75K
		gl	25	0.10	NaClO <sub>4</sub>	4.86	4.86						58W
		gl	25	0.10	NaClO <sub>4</sub>	5.06	5.06	2.60	2.60			MHL + HL = 2.67	67S
		gl	25	0.10	NaNO <sub>3</sub>	4.97	4.97	2.8	2.8				86C
		gl	25	0.12	NaCl	4.54	4.58					large [M]/[L]?	87S
		ix	?	0.25	NaCl	3.74	4.0					large [M]/[L]?	78R
												sulfate, T = ?	85J
												pH=7.5, buffer	
Ni <sup>2+</sup>		gl	30	0.10	Me <sub>4</sub> NBr	5.32	5.30	2.98	2.97				66Pa
		gl	22?	0.10	KCl	4.61	4.63					sulfate, large [L]	60B
		gl	22	0.10	KCl	4.54	4.56					ML-H = -9.3, sulfate large [L]	61B
		kin	25	0.10	KNO <sub>3</sub>	5.0	5.0						64H
		gl	0	0.10	KNO <sub>3</sub>	5.18		2.88					66T
		gl	12	0.10	KNO <sub>3</sub>	5.05		2.80					66T
		gl	25	0.10	KNO <sub>3</sub>	5.02	5.02	2.72	2.72				62T
		gl	25	0.10	KNO <sub>3</sub>	4.83		2.31				large [M]/[L]	66
		gl	40	0.10	KNO <sub>3</sub>	4.90		2.59					62T
		gl	15	0.10	KNO <sub>3</sub>	4.79	4.83	2.78	2.80				66T
		sp	15	0.10	KNO <sub>3</sub>							ML + M = 2.40	72F
		gl	25	0.10	KCl	4.57	4.57	2.61	2.61				72Fa
		gl	25	0.10	NaClO <sub>4</sub>	4.85	4.85						80D
		gl	25	0.10	NaClO <sub>4</sub>							ML-H = -9.41	67S
		gl	25	0.10	NaNO <sub>3</sub>	4.86	4.86	2.86	2.86				75S
		gl	25	0.12	NaCl	4.50	4.54					large [M]/[L]?	87S
Cu <sup>2+</sup>		gl	30	0.10	Me <sub>4</sub> NBr	6.83	6.82	3.79	3.79				78R
		gl	25	0.10	K <sup>+</sup> corr	6.50	6.50	2.92	2.92			ML + L = 2.0 ML + M = 2.26 MHL + M = 2.1 2MOHL = 1.8 ML-H = -6.8	66Pa
		gl	22?	0.10	KCl	5.50	5.51					sulfate, large [L]	60B
		gl	22	0.10	KCl	5.77	5.78					ML-H = -7.7, sulfate large [L]	61B
		gl	20	0.10	KCl	5.82	5.83	3.25	3.25	1.94	1.88	ML + M = 1.88 large [M]/[L]	62H
		gl	0	0.10	KNO <sub>3</sub>	6.42		3.32				ML-H = -7.05 MOHL-H = -7.32	66T
		gl	12	0.10	KNO <sub>3</sub>	6.20		3.20				2MOHL = 3.10 ML-H = -6.74 2MOHL = 2.80	66T

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.			
ATP	Cu <sup>2+</sup>	gl	25	0.10	KNO <sub>3</sub>	6.13	6.13	3.12	3.12			ML-H = -6.47 MOHL-H = -7.03 2MOHL = 2.59	62T 66T			
		gl	25	0.10	KNO <sub>3</sub>	6.01		2.78				large [M]/[L]	62T			
		gl	40	0.10	KNO <sub>3</sub>	5.97		3.01					ML-H = -6.19 MOHL-H = -6.91 2MOHL = 2.38	66T		
		gl	35	0.10	KNO <sub>3</sub>	6.34	6.32	3.59	3.59					79Mc		
		gl	25	0.10	KCl	6.08	6.08	3.62	3.62					80D		
		gl	25	0.10	KNO <sub>3</sub>	5.83	5.83	2.91	2.91				ML + M = 2.36 MHL + M = 2.1 ML-H = -6.65 2MOHL = 2.29 M <sub>2</sub> L-H = -4.9	83A		
		gl	25	0.10	KNO <sub>3</sub>	6.46	6.46	3.43	3.43				ML + L = 2.77 ML-H = -8.01 MOHL + M = 5.09 large HL const.	86C		
		gl	22	0.25	KNO <sub>3</sub>	6.0	6.3							84G		
		gl	25	1.00	KNO <sub>3</sub>	5.17								76R		
		gl	20	0.10	NaClO <sub>4</sub>	6.30	6.31	3.76	3.72					64Sa		
		gl	25	0.10	NaClO <sub>4</sub>	6.38	6.38							67S		
		gl	25	0.10	NaClO <sub>4</sub>								ML-H = -7.9	68S		
		gl	25	0.10	NaClO <sub>4</sub>	6.03	6.03							78M		
		gl	20	0.10	NaNO <sub>3</sub>	6.10	6.11	3.45	3.41				ML-H = -8.09 2M + 2L-H = -6.85 M <sub>2</sub> OHL <sub>2</sub> -H = -8.04 ML + L = 1.8 ML <sub>2</sub> -3H = -30.9 M(OH) <sub>3</sub> L <sub>2</sub> -H = -10.5 2M + 2L-H = -6.9 M <sub>2</sub> OHL <sub>2</sub> -H = -8.6M M <sub>2</sub> (OH) <sub>2</sub> L <sub>2</sub> -H = -10 M <sub>2</sub> (OH) <sub>3</sub> L <sub>2</sub> -H = -12	83W		
		epr	20	0.10	NaNO <sub>3</sub>	6.2		3.4							83W	
		Zn <sup>2+</sup>		gl	25	0.10	NaNO <sub>3</sub>	6.32	6.32	3.57	3.57					85T
				gl	25	0.10	NaClO <sub>4</sub>	6.51	6.51	3.61	3.61				ML-H = -7.72	86C
				gl	25	0.10	NaNO <sub>3</sub>	6.34	6.34	3.59	3.59					87S
				gl	25	0.12	NaCl	6.0	6.0						large [M]/[L]?	78R
				gl	30	0.10	Me <sub>4</sub> NBr	5.52	5.47	2.91	2.89					66Pa
gl	25			0.10	K <sup>+</sup> corr	5.23	5.23	2.12	2.12				ML + L = 1.9 ML + M = 1.85 MHL + M = 2.0 ML-H = -8.4 M <sub>2</sub> L-H = -7.0	83A		
gl	25			0.10	KCl	4.76	4.76	2.75	2.75				large [M]/[L]	58Wa		
gl	22			0.10	KCl	4.80	4.83						ML-H = -8.5, sulfate large [L]	61B		
gl	20			0.10	KCl	4.75	4.80	2.78	2.09	2.09	2.03		ML + M = 1.41 large [M]/[L]	62H		
gl	0			0.10	KNO <sub>3</sub>	5.00		2.81						66T		
gl	12			0.10	KNO <sub>3</sub>	4.88		2.73						66T		
gl	25			0.10	KNO <sub>3</sub>	4.85	4.85	2.67	2.67					62T		
gl	25			0.10	KNO <sub>3</sub>	4.75		2.23					large [M]/[L]	66T		
gl	40			0.10	KNO <sub>3</sub>	4.71		2.58						66T		
gl	35			0.10	KNO <sub>3</sub>	5.25	5.15	2.68	2.64					79Mc		
gl	25			0.10	KCl	4.92	4.92	2.94	2.94					80Db		
gl	25			0.10	KNO <sub>3</sub>	4.66	4.66	2.08	2.08				ML + M = 1.85 ML-H = -8.5 MHL + M = 2.0 M <sub>2</sub> L-H = -7.0	83A		
gl	25			0.10	KNO <sub>3</sub>	4.92	4.92							85M		
gl	25			0.10	KNO <sub>3</sub>	5.44	5.44	3.12	3.12	2.37			ML + L = 2.46 ML + M = 1.78 M <sub>2</sub> L-H = -5.94 large HL const.	86C		
gl	22			0.25	KNO <sub>3</sub>	5.65	5.97							84G		
gl	25	1.00	KNO <sub>3</sub>	3.2								76R				
ix	18	0.05	NaClO <sub>4</sub>	7.26	7.21							78K				
gl	25	0.10	NaClO <sub>4</sub>	5.21	5.21							67S				

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
<b>ATP</b>													
Zn <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.87	75S
	gl		25	0.10	NaClO <sub>4</sub>	5.10	5.10						78M
	gl		25	0.10	NaClO <sub>4</sub>	5.81	5.81	3.62	3.62	3.14		ML+L = 2.46 ML-H = -8.4 ML+M = 2.45 MHL+M = 1.8 M <sub>2</sub> L-H = -6.70	86C
	gl		25	0.10	NaNO <sub>3</sub>	5.16	5.16	2.86	2.86				87S
	gl		25	0.12	NaCl	4.1	4.1					large [M]/[L]?	78R
	ix		?	0.25	NaCl	3.68	4.0					pH = 7.5, buffer	85J
Cd <sup>2+</sup>	gl		22?	0.10	KCl	4.70	4.73					sulfate, large [L]	60B
	nmr		30	0.10	KNO <sub>3</sub>	4.4		1.9				large [L]	84P
	gl		30	1.00	KNO <sub>3</sub>	5.41		2.70				wrong HL const.	84C
	gl		25	0.10	NaNO <sub>3</sub>	5.31	5.31	2.95	2.95			ML-H = -10.1	84Sa
	gl		25	0.10	NaNO <sub>3</sub>	5.34	5.34	3.04	3.04				87S
	nmr		32	1.5	CdCl <sub>2</sub>	5.19		4.25		3.03		large [L]	85B
<b>GTP</b>													
Mn <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	5.18	5.18						73T
	gl		35	0.10	KNO <sub>3</sub>	5.29							73T
	gl		45	0.10	KNO <sub>3</sub>	5.09							73T
	ix		23	0.10	NaCl	4.73	4.75					TRIS buffer large [M]/[L] pH = 8.2	58W
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -9.36 MOHL-H = -11.3	75S
Co <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.64	4.64						77S
	gl		25	0.10	KNO <sub>3</sub>	5.57	5.57						73T
	gl		35	0.10	KNO <sub>3</sub>	5.65							73T
	gl		45	0.10	KNO <sub>3</sub>	5.50							73T
	ix		23	0.10	NaCl	4.63	4.65					TRIS buffer large [M]/[L] pH = 8.2	58W
Ni <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	5.78	5.78						73T
	gl		35	0.10	KNO <sub>3</sub>	5.87							73T
	gl		45	0.10	KNO <sub>3</sub>	5.70							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.64 MOHL-H = -10.57	75S
Cu <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	6.55	6.55						73T
	gl		35	0.10	KNO <sub>3</sub>	6.66							73T
	gl		45	0.10	KNO <sub>3</sub>	6.35							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -7.7 MOHL-H = -9.3 ML-H = -7.5	68S
	sp		25	0.10	NaClO <sub>4</sub>								68S
Zn <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	5.93	5.93						77S
	gl		25	0.10	NaClO <sub>4</sub>	5.93	5.93						77S
	gl		25	0.10	KNO <sub>3</sub>	5.72	5.72						73T
	gl		35	0.10	KNO <sub>3</sub>	5.76							73T
	gl		45	0.10	KNO <sub>3</sub>	5.64							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.39, MOHL-H = -9.48	75S
	gl		25	0.10	NaClO <sub>4</sub>	4.96	4.96						77S
<b>ITP</b>													
Mn <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	4.45	4.45						73T
	gl		35	0.10	KNO <sub>3</sub>	4.62							73T
	gl		45	0.10	KNO <sub>3</sub>	4.35							73T
	ix		23	0.10	NaCl	4.57	4.59					TRIS buffer large [M]/[L] pH = 8.2	58W
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.93 MOHL-H = -11.2	75S
Co <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.66	4.66						77Sa
	gl		25	0.10	KNO <sub>3</sub>	4.97	4.97						73T
	gl		35	0.10	KNO <sub>3</sub>	5.02							73T
	gl		45	0.10	KNO <sub>3</sub>	4.92							73T
	ix		23	0.10	NaCl	4.74	4.76					pH = 8.2, TRIS buffer large [M]/[L]	58W
	gl		25	0.10	NaClO <sub>4</sub>	4.81	4.81						77C



Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
<b>ITP</b>													
Ni <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	5.06	5.06						73T
	gl		35	0.10	KNO <sub>3</sub>	5.12							73T
	gl		45	0.10	KNO <sub>3</sub>	5.01							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.39, MOHL-H = -10.6	75S
Cu <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.73	4.73						77C
	gl		25	0.10	KNO <sub>3</sub>	5.76	5.76						73T
	gl		35	0.10	KNO <sub>3</sub>	5.92							73T
	gl		45	0.10	KNO <sub>3</sub>	5.56							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -7.5, MOHL-H = -9.2	68S
Zn <sup>2+</sup>	sp		25	0.10	NaClO <sub>4</sub>							ML-H = -7.2	68S
	gl		25	0.10	NaClO <sub>4</sub>	5.99	5.99						77C
	gl		25	0.10	KNO <sub>3</sub>	4.57	4.57						73T
	gl		35	0.10	KNO <sub>3</sub>	4.77							73T
	gl		45	0.10	KNO <sub>3</sub>	4.50							73T
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.31, MOHL-H = -9.4	75S
<b>CTP</b>													
Mn <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	5.02	5.02						77C
	gl		25	0.10	KNO <sub>3</sub>	4.56	4.56	4.24	4.24				83R
	gl		35	0.10	KNO <sub>3</sub>	4.43		4.10					75T
Co <sup>2+</sup>	gl		45	0.10	KNO <sub>3</sub>	4.85		4.01					83R
	gl		25	0.10	KCl	4.63	4.63	2.5	2.5				84M
	ix		23	0.10	NaCl	4.78	4.80					TRIS buffer, large [M]/[L] pH = 8.2	58W
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -10.9	75S
	gl		25	0.10	NaClO <sub>4</sub>	4.74	4.74						77S
	gl		25	0.10	NaNO <sub>3</sub>	4.90	4.90	3.1	3.1				87S
	gl		25	0.10	KNO <sub>3</sub>	5.07	5.07	4.45	4.45				83R
	gl		35	0.10	KNO <sub>3</sub>	4.96		4.36					75T
	gl		45	0.10	KNO <sub>3</sub>	4.32(?)		4.25					83R
	gl		25	0.10	KCl	4.69	4.69	2.58	2.58				84M
ix		23	0.10	NaCl	4.48	4.50					TRIS buffer large [M]/[L] pH = 8.2	58W	
Ni <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	4.78	4.78	3.0	3.0				87S
	gl		15	0.10	KNO <sub>3</sub>	4.41	4.49	2.68	2.74				72F
	sp		15	0.10	KNO <sub>3</sub>							ML + M = 2.23	78F
	gl		25	0.10	KNO <sub>3</sub>	5.69	5.69	4.74	4.74				83R
	gl		35	0.10	KNO <sub>3</sub>	5.58	4.61						75T
Cu <sup>2+</sup>	gl		45	0.10	KNO <sub>3</sub>	5.51	4.51						83R
	gl		25	0.10	KCl	4.51	4.51	2.7	2.7				84M
	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -9.6	75S
	gl		25	0.10	NaNO <sub>3</sub>	4.52	4.52	2.7	2.7				87S
	gl		25	0.10	KNO <sub>3</sub>	6.73	6.73	5.56	5.56				83R
	gl		35	0.10	KNO <sub>3</sub>	6.61		5.45					75T
	gl		45	0.10	KNO <sub>3</sub>	6.50		5.36					83R
	gl		25	0.10	KCl	5.64	5.64	3.42	3.42				84M
Zn <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -7.6	68S
	gl		25	0.10	NaClO <sub>4</sub>	5.7	5.7						77S
	gl		25	0.10	NaNO <sub>3</sub>	6.03	6.03	3.80	3.80				87S
	gl		25	0.10	KNO <sub>3</sub>	5.22	5.22	4.56	4.56				83R
	gl		35	0.10	KNO <sub>3</sub>	5.12		4.48					75T
	gl		45	0.10	KNO <sub>3</sub>	5.02		4.40					83R
	gl		25	0.10	KCl	4.79	4.79	2.9	2.9				84M
Cd <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>							ML-H = -8.79	75S
	gl		25	0.10	NaClO <sub>4</sub>	4.79	4.79						77S
	gl		25	0.10	NaNO <sub>3</sub>	5.03	5.03	3.05	3.05				87S
	gl		25	0.10	NaNO <sub>3</sub>	4.99	4.99	3.16	3.16				84Sa
	gl		25	0.10	NaNO <sub>3</sub>	5.05	5.05	3.15	3.15				87S
	gl		25	0.10	NaNO <sub>3</sub>							ML-H = -10.0	84Sa

Table 3. (continued)

<u>Ligand</u>	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.
<u>UTP</u> Mn <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	6.31	6.31						83R
	gl		35	0.10	KNO <sub>3</sub>	6.21							76T
	gl		45	0.10	KNO <sub>3</sub>	6.10							83R
	ix		23	0.10	NaCl	4.78	4.80					TRIS buffer large [M]/[L] pH=8.2	83R
	gl		25	0.10	NaClO <sub>4</sub>							MOHL-H=-11.1	75S
Co <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.58	4.58						77S
	gl		25	0.10	NaNO <sub>3</sub>	4.91	4.91	2.70	2.70				87S
	gl		25	0.10	KNO <sub>3</sub>	6.94	6.94						83R
	gl		35	0.10	KNO <sub>3</sub>	6.84							76T
	gl		35	0.10	KNO <sub>3</sub>	6.84							83R
	ix		45	0.10	KNO <sub>3</sub>	6.01(?)							83R
	ix		23	0.10	NaCl	4.55	4.57					TRIS buffer large [M]/[L] pH=8.2	58W
Ni <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.53	4.53						78F
	gl		25	0.10	NaNO <sub>3</sub>	4.73	4.73	2.6	2.6				87S
	gl		25	0.10	KNO <sub>3</sub>	7.67	7.67						83R
	gl		35	0.10	KNO <sub>3</sub>	7.56							76T
	gl		45	0.10	KNO <sub>3</sub>	7.44							83R
	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-9.10	83R
												MOHL-H=-9.7	75S
Cu <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.29	4.29						78F
	gl		25	0.10	NaNO <sub>3</sub>	4.47	4.47	2.5	2.5				87S
	gl		25	0.10	KNO <sub>3</sub>	8.99	8.99						83R
	gl		35	0.10	KNO <sub>3</sub>	8.88							76T
	gl		45	0.10	KNO <sub>3</sub>	8.76							83R
	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-7.8	83R
												MOHL-H=-8.4	68S
												ML-H=-7.8	68S
Zn <sup>2+</sup>	sp		25	0.10	NaClO <sub>4</sub>								68S
	gl		25	0.10	NaClO <sub>4</sub>	5.53	5.53						78F
	gl		25	0.10	NaNO <sub>3</sub>	5.81	5.81	2.8	2.8				85T
	gl		25	0.10	NaNO <sub>3</sub>	5.87	5.87	2.80	2.80				87S
	gl		25	0.10	KNO <sub>3</sub>	7.21	7.21						83R
	gl		35	0.10	KNO <sub>3</sub>	7.10							76T
	gl		45	0.10	KNO <sub>3</sub>	7.00							83R
	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-8.71	75S
												MOHL-H=-9.24	
Cd <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.75	4.75						78F
	gl		25	0.10	NaNO <sub>3</sub>	5.01	5.01	2.73	2.73				87S
	gl		25	0.10	NaNO <sub>3</sub>	5.10	5.10	2.89	2.89				87S
<u>ITP</u> Mn <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-9.67	75S
												MOHL-H=-11.2	
Co <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	5.0	5.0						87S
	gl		25	0.10	NaNO <sub>3</sub>	4.78	4.78						87S
Ni <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-9.08	75S
												MOHL-H=-9.9	
Cu <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	4.52	4.52						87S
	gl		25	0.10	NaClO <sub>4</sub>	5.70	5.70						77S
	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-7.7	68S
												MOHL-H=-8.2	
												ML-H=-7.9	68S
Zn <sup>2+</sup>	sp		25	0.10	NaClO <sub>4</sub>								68S
	gl		25	0.10	NaNO <sub>3</sub>	5.8	5.8						87S
	gl		25	0.10	NaClO <sub>4</sub>							ML-H=-8.35	75S
												MOHL-H=-9.2	
Cd <sup>2+</sup>	gl		25	0.10	NaClO <sub>4</sub>	4.89	4.89						77S
	gl		25	0.10	NaNO <sub>3</sub>	5.03	5.03						87S
	gl		25	0.10	NaNO <sub>3</sub>	5.09	5.09						87S

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Ref.	
ADP Mn <sup>2+</sup>	gl		25	0.20	Pr <sub>4</sub> NCl	3.54	3.64	1.49	1.53				56Sa	
	gl		0	0.20	Me <sub>4</sub> NBr	4.24						assume [H] = [Mn] pH=7.5	77R	
	gl		8	0.20	Me <sub>4</sub> NBr	4.24						assume [H] = [Mn] pH=7.5	77R	
	gl		15	0.20	Me <sub>4</sub> NBr	4.23						assume [H] = [Mn] pH=7.5	77R	
	gl		25	0.20	Me <sub>4</sub> NBr	4.31	4.41					assume [H] = [Mn] pH=7.5	77R	
	gl		35	0.20	Me <sub>4</sub> NBr	4.40						assume [H] = [Mn] pH=7.5	77R	
	gl		45	0.20	Me <sub>4</sub> NBr	4.47						assume [H] = [Mn] pH=7.5	77R	
	epr		2	0.0085	NEM.HCl	4.91						pH=8.0, buffer	70J	
	epr		12	0.0085	NEM.HCl	4.95						pH=8.0, buffer	70J	
	epr		25	0.0085	NEM.HCl	4.98	4.31					pH=8.0, buffer	70J	
	epr		32	0.0085	NEM.HCl	5.06						pH=8.0, buffer	70J	
	epr		47	0.0085	NEM.HCl	5.17						pH=8.0, buffer	70J	
	sp		30	0.02	NEM.HCl	4.40	4.16					pH=8.0, buffer	640	
	epr		27	0.02	NEM.HCl	4.48	4.22					pH=8.0, buffer	640	
	gl		0	0.10	KNO <sub>3</sub>	4.47		2.00						67T
	gl		12	0.10	KNO <sub>3</sub>	4.24		1.95						67T
	gl		25	0.10	KNO <sub>3</sub>	4.16	4.16	1.89	1.89					62Ta
	gl		40	0.10	KNO <sub>3</sub>	4.06		1.81						67T
	gl		25	0.10	KCl	3.80	3.80	2.37	2.37					80Db
	epr		37	0.15	KCl	4.05	4.02						BIS-TRIS buffer pH=7.2	78Gb
	gl		22	0.25	KNO <sub>3</sub>	3.0	3.2						large HL const.	84G
	ix		23	0.10	NaCl	3.94	3.96						pH=8.2, TRIS buffer, large [M]/[L]	58W
	epr		25	0.11	NaCl	4.20	4.20						pH=8.0, NEM buffer	70J
	ix		26	0.11	NaCl	4.15	4.15						pH=8.0, NEM buffer	70J
	ix		41	0.11	NaCl	4.30							pH=8.0, NEM buffer	70J
	ix		?	dilute	?	3.28							few details, T=?	80K
	Co <sup>2+</sup>	gl		5	0.20	Me <sub>4</sub> NBr	3.87						pH=?	
gl			15	0.20	Me <sub>4</sub> NBr	3.88						pH=6.0	80M	
gl			25	0.20	Me <sub>4</sub> NBr	3.94						pH=6.0	80M	
gl			37	0.20	Me <sub>4</sub> NBr	4.02						pH=6.0	80M	
gl			25	0.20	Me <sub>4</sub> NBr	3.81	3.88	2.71	2.75			ML+L=2.18	80M	
gl			0	0.10	KNO <sub>3</sub>	4.63		2.12					67T	
gl			12	0.10	KNO <sub>3</sub>	4.27		2.07					67T	
gl			25	0.10	KNO <sub>3</sub>	4.20	4.20	2.01	2.01				62Ta	
gl			40	0.10	KNO <sub>3</sub>	4.12		1.93					67T	
gl			25	0.10	KCl	3.51	3.51	1.87	1.87				80Da	
ix			20	0.05	NaClO <sub>4</sub>	6.12	6.12					large [L]	75K	
ix			23	0.10	NaCl	3.68	3.70					TRIS buffer, large [M]/[L] pH=8.2	58W	
Ni <sup>2+</sup>		gl		5	0.20	Me <sub>4</sub> NBr	3.99						pH=constant	79M
	gl		15	0.20	Me <sub>4</sub> NBr	3.98						pH=constant	79M	
	gl		25	0.20	Me <sub>4</sub> NBr	4.00						pH=constant	79M	
	gl		37	0.20	Me <sub>4</sub> NBr	4.04						pH=constant	79M	
	gl		25	0.20	Me <sub>4</sub> NBr	3.90	3.97	2.28	2.32			ML+L=2.25	79M	
	cal		25	0.20	Me <sub>4</sub> NBr	4.2							79M	
	gl		0	0.10	KNO <sub>3</sub>	4.62		2.43					67T	
	gl		12	0.10	KNO <sub>3</sub>	4.57		2.37					67T	
	gl		25	0.10	KNO <sub>3</sub>	4.50	4.50	2.30	2.30				62Ta	
	gl		40	0.10	KNO <sub>3</sub>	4.42		2.22					67T	
	gl		15	0.10	KNO <sub>3</sub>	4.18	4.22	2.30	2.32			ML+L=2.30	72F	
	gl		15	0.10	KNO <sub>3</sub>							ML+M=1.60	72Fa	
	gl		25	0.10	KNO <sub>3</sub>	3.71	3.71	2.10	2.10				80D	

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Remarks	Ref.
<b>ADP</b>														
Cu <sup>2+</sup>	gl		0	0.10	KNO <sub>3</sub>	6.16		2.80					ML-H = -7.65 2MOHL = 3.85	67T
	gl		12	0.10	KNO <sub>3</sub>	6.04		2.72					ML-H = -7.38, 2MOHL = 3.65	67T
	gl		25	0.10	KNO <sub>3</sub>	5.90	5.90	2.63	2.63				ML-H = -7.08 2MOHL = 3.42	62Ta 67T
	gl		40	0.10	KNO <sub>3</sub>	5.75		2.52					ML-H = -6.76 2MOHL = 3.19	67T
	gl		25	0.10	KCl	5.38	5.38	2.94	2.94					80D
Zn <sup>2+</sup>	gl		22	0.25	KNO <sub>3</sub>	4.6	4.8						large HL const.	84G
	gl		25	0.10	KCl	4.13	4.13	2.34	2.34					58Wa
	gl		0	0.10	KNO <sub>3</sub>	4.40		2.15					ML-H = -9.14, 2MOHL = 3.66	67T
	gl		12	0.10	KNO <sub>3</sub>	4.35		2.11					ML-H = -8.83, 2MOHL = 3.50	67T
	gl		25	0.10	KNO <sub>3</sub>	4.28	4.28	2.04	2.04				ML-H = -8.51 2MOHL = 3.34	62Ta 67T
	gl		40	0.10	KNO <sub>3</sub>	4.20		1.96					ML-H = -8.18, 2MOHL = 3.16	67T
	gl		25	0.10	KCl	4.17	4.17	2.44	2.44					80Db
	gl		22	0.25	KNO <sub>3</sub>	4.4	4.6						large HL const.	84G
	nmr		30	0.10	KNO <sub>3</sub>	3.6		1.7					large [L]	84P
<b>Cd<sup>2+</sup></b>														
<b>CDP</b>														
Mn <sup>2+</sup>	gl		25	0.10	KCl	3.82	3.82	1.8	1.8				small HL const.	84M
Co <sup>2+</sup>	gl		25	0.10	KCl	3.87	3.87	2.4	2.4				small HL const.	84M
Ni <sup>2+</sup>	gl		15	0.10	KNO <sub>3</sub>	3.48	3.52	1.87	1.89				ML + L = 1.99	72F
	sp		15	0.10	KNO <sub>3</sub>								ML + M = 1.70	72Fa
	gl		25	0.10	KCl	3.82	3.82	2.3	2.3				small HL const.	84M
Cu <sup>2+</sup>	gl		25	0.10	KCl	4.89	4.89	2.7	2.7				small HL const.	84M
Zn <sup>2+</sup>	gl		25	0.10	KCl	3.93	3.93	2.47	2.47				small HL const.	84M
<b>AMP-5</b>														
Mn <sup>2+</sup>	gl		25	0.20	Pr <sub>4</sub> NBr	2.19	2.23							56Sa
	gl		0	0.20	Me <sub>4</sub> NBr	2.46							assume [H] = [Mn] pH = 7.0	77R
	gl		8	0.20	Me <sub>4</sub> NBr	2.35							assume [H] = [Mn] pH = 7.0	77R
	gl		15	0.20	Me <sub>4</sub> NBr	2.28							assume [H] = [Mn] pH = 7.0	77R
	gl		25	0.20	Me <sub>4</sub> NBr	2.33	2.37						assume [H] = [Mn] pH = 7.0	77R
	gl		35	0.20	Me <sub>4</sub> NBr	2.27(?)							assume [H] = [Mn] pH = 7.0	77R
	gl		45	0.20	Me <sub>4</sub> NBr	2.39							assume [H] = [Mn] pH = 7.0	77R
	gl		0	0.10	KNO <sub>3</sub>	2.46								67T
	gl		12	0.10	KNO <sub>3</sub>	2.43								67T
	gl		25	0.10	KNO <sub>3</sub>	2.40	2.40							62Ta 67T
	gl		40	0.10	KNO <sub>3</sub>	2.37								67T
	gl		25	0.10	KNO <sub>3</sub>	2.35	2.35							66D
	gl		25	0.10	KCl	2.02	2.02							80Db
	ix		23	0.10	NaCl	2.31	2.32						TRIS buffer large [M]/[L] pH = 8.2	58W
	ix		25	0.10	NaEt <sub>2</sub> Bar.	2.19	2.19						barbiturate buffer pH = 6.9	61T
	gl		25	0.10	NaClO <sub>4</sub>	2.14	2.14						large [M]/[L]	64S
	gl		25	0.10	NaNO <sub>3</sub>	2.23	2.23						large [M]/[L]	88Sa
	gl		5	0.20	Me <sub>4</sub> NBr	2.46							assume [H] = [Co] pH = 7.0	80M
	gl		15	0.20	Me <sub>4</sub> NBr	2.38							assume [H] = [Co] pH = 7.0	80M
	gl		25	0.20	Me <sub>4</sub> NBr	2.35							assume [H] = [Co] pH = 7.0	80M
	gl		37	0.20	Me <sub>4</sub> NBr	2.37							assume [H] = [Co] pH = 7.0	80M
	gl		25	0.20	Me <sub>4</sub> NBr	2.32	2.36							80M
	cal		25	0.20	Me <sub>4</sub> NBr	2.35							pH = 7.0	80M



Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Remarks	Ref.
<b>AMP-3</b>														
Co <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	2.06	2.06						large [M]/[L]	89M
	gl		25	0.10	Me <sub>4</sub> NBr	2.19	2.19	0.2	0.2					66D
	gl		25	0.10	KNO <sub>3</sub>	2.10	2.10							66D
	ix		25	0.10	KClO <sub>4</sub>	2.08								66D
	gl		0	0.10	KNO <sub>3</sub>	2.11								67T
	gl		12	0.10	KNO <sub>3</sub>	2.15								67T
	gl		25	0.10	KNO <sub>3</sub>	2.20	2.20							62Ta
Ni <sup>2+</sup>	gl		40	0.10	KNO <sub>3</sub>	2.24								67T
	gl		25	0.10	NaNO <sub>3</sub>	1.80	1.80						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	2.85								67T
	gl		12	0.10	KNO <sub>3</sub>	2.82								67T
	gl		25	0.10	KNO <sub>3</sub>	2.79	2.79							62Ta
														67T
														67T
Cu <sup>2+</sup>	gl		40	0.10	KNO <sub>3</sub>	2.75								67T
	gl		15	0.10	KNO <sub>3</sub>	2.08	2.02	0.7	0.7					80Ta
	gl		25	0.10	NaClO <sub>4</sub>	1.98	1.98	1.1	1.1					76Ta
	gl		25	0.10	NaNO <sub>3</sub>	1.89	1.89						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	3.06								67T
	gl		12	0.10	KNO <sub>3</sub>	3.00								67T
	gl		25	0.10	KNO <sub>3</sub>	2.96	2.96							62Ta
Zn <sup>2+</sup>														67T
	gl		40	0.10	KNO <sub>3</sub>	2.90								67T
	gl		25	0.10	NaNO <sub>3</sub>	2.75	2.75						large [M]/[L]	89M
	gl		25	0.10	KCl	2.69	2.69							58Wa
	ix		25	0.10	KClO <sub>4</sub>	2.48	2.48							66D
	gl		0	0.10	KNO <sub>3</sub>	2.65								67T
	gl		12	0.10	KNO <sub>3</sub>	2.62								67T
Cd <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	2.60	2.60							62Ta
	gl		40	0.10	KNO <sub>3</sub>	2.56								67T
	gl		25	0.10	NaNO <sub>3</sub>	1.98	1.98						large [M]/[L]	89M
AMP-2	gl		25	0.10	NaNO <sub>3</sub>	2.32	2.32						large [M]/[L]	89M
	gl		25	0.10	NaNO <sub>3</sub>	2.32	2.32							89M
	gl		25	0.10	NaNO <sub>3</sub>	2.32	2.32							89M
Mn <sup>2+</sup>	gl		0	0.10	KNO <sub>3</sub>	2.43								67T
	gl		12	0.10	KNO <sub>3</sub>	2.41								67T
	gl		25	0.10	KNO <sub>3</sub>	2.38	2.38							67T
	gl		40	0.10	KNO <sub>3</sub>	2.35								67T
	gl		25	0.10	NaNO <sub>3</sub>	2.14	2.14						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	2.15								67T
	gl		12	0.10	KNO <sub>3</sub>	2.19								67T
Co <sup>2+</sup>	gl		25	0.10	KNO <sub>3</sub>	2.24	2.24							67T
	gl		40	0.10	KNO <sub>3</sub>	2.28								67T
	gl		25	0.10	NaNO <sub>3</sub>	1.93	1.93						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	2.86								67T
	gl		12	0.10	KNO <sub>3</sub>	2.84								67T
	gl		25	0.10	KNO <sub>3</sub>	2.81	2.81							67T
	gl		40	0.10	KNO <sub>3</sub>	2.78								67T
Ni <sup>2+</sup>	gl		15	0.10	KNO <sub>3</sub>	2.08	2.02						ML+L=2.20	72F
	gl		15	0.10	KNO <sub>3</sub>	2.18	2.12	0.7	0.7				ML+L=1.40	80Ta
	gl		25	0.10	NaNO <sub>3</sub>	1.94	1.94						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	3.28								67T
	gl		12	0.10	KNO <sub>3</sub>	3.23								67T
	gl		25	0.10	KNO <sub>3</sub>	3.16	3.16							67T
	gl		40	0.10	KNO <sub>3</sub>	3.10								67T
Cu <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	3.01	3.01						large [M]/[L]	89M
	gl		0	0.10	KNO <sub>3</sub>	2.72								67T
	gl		12	0.10	KNO <sub>3</sub>	2.68								67T
	gl		25	0.10	KNO <sub>3</sub>	2.64	2.64							67T
	gl		40	0.10	KNO <sub>3</sub>	2.60								67T
	gl		25	0.10	NaNO <sub>3</sub>	2.10	2.10						large [M]/[L]	89M
	gl		25	0.10	NaNO <sub>3</sub>	2.41	2.41						large [M]/[L]	89M
Cd <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	2.41	2.41							89M
	gl		25	0.10	NaNO <sub>3</sub>	2.41	2.41							89M
<b>GMP-5</b>														
Cu <sup>2+</sup>	gl		37	0.15	NaCl								2M+3H+2L=34.67 M <sub>2</sub> H <sub>3</sub> L <sub>2</sub> +H=3.15	83C
Cd <sup>2+</sup>	gl		25	0.10	NaNO <sub>3</sub>	2.98	2.98						large [M]/[L]	88Ma
<b>IMP-5</b>														
Ni <sup>2+</sup>	sp		15	0.20	NaClO <sub>3</sub>	2.96	2.91	1.88	1.8				ML-H=-7.96	81N

Table 3. (continued)

Ligand		Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
<b>CMP-5</b>														
	Mn <sup>2+</sup>	gl	25	0.10	KCl	2.4	2.4							84M
		gl	35	0.10	KNO <sub>3</sub>	2.65	2.59							85K
	Co <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.10	2.10						large [M]/[L]	88M
		gl	25	0.10	KCl	2.3	2.3							84M
		gl	35	0.10	KNO <sub>3</sub>	3.50	3.50(?)							85K
	Ni <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.86	1.86						large [M]/[L]	88M
		gl	15	0.10	KNO <sub>3</sub>	1.90	1.84	0.5	0.5					72F
														80T
		gl	25	0.10	KNO <sub>3</sub>	2.00	2.00							80O
		gl	25	0.10	KCl	2.2	2.2							84M
		gl	35	0.10	KNO <sub>3</sub>	2.36	2.42							85K
	Cu <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.94	1.94						large [M]/[L]	88M
		gl	25	0.10	KCl	3.2	3.2							84M
		gl	35	0.10	KNO <sub>3</sub>	3.90	4.00(?)							85K
	Zn <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.84	2.84						large [M]/[L]	88M
		gl	25	0.10	KCl	2.54	2.54							58Wa
		gl	25	0.10	KCl	2.6	2.6							84M
		gl	35	0.10	KNO <sub>3</sub>	2.25	2.27							85K
	Cd <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.06	2.06						large [M]/[L]	88M
		gl	25	0.10	NaNO <sub>3</sub>	2.40	2.40						large [M]/[L]	88M
<b>UMP-5</b>														
	Mn <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.01	2.01						large [M]/[L]	84S
		gl	25	0.10	NaNO <sub>3</sub>	2.11	2.11						large [M]/[L]	88M
	Co <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.87	1.87						large [M]/[L]	88M
	Ni <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.97	1.97						large [M]/[L]	88M
	Cu <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.80	2.80						large [M]/[L]	84S
		gl	25	0.10	NaNO <sub>3</sub>	2.77	2.77						large [M]/[L]	88M
	Zn <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.03	2.03						large [M]/[L]	84S
		gl	25	0.10	NaNO <sub>3</sub>	2.02	2.02						large [M]/[L]	88M
	Cd <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.38	2.38						large [M]/[L]	88M
<b>TMP-5</b>														
	Mn <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.11	2.11						large [M]/[L]	88M
	Co <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.89	1.89						large [M]/[L]	88M
	Ni <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	1.92	1.92						large [M]/[L]	88M
	Cu <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.87	2.87						large [M]/[L]	88M
	Zn <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.10	2.10						large [M]/[L]	88M
	Cd <sup>2+</sup>	gl	25	0.10	NaNO <sub>3</sub>	2.42	2.42						large [M]/[L]	88M
<b>ATP</b>														
	Be <sup>2+</sup>	gl	22?	0.10	KCl	5.01							sulfate, large [L]	60B
	Sc <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.35							pH=8.0, buffer	83M
	Y <sup>3+</sup>	gl	9	0.10	NaClO <sub>4</sub>	6.44				3.88				82Sa
		gl	17	0.10	NaClO <sub>4</sub>	6.30				3.71				82Sa
		gl	25	0.10	NaClO <sub>4</sub>	6.29	6.29			3.64	3.64			82Sa
														87Sa
		gl	32	0.10	NaClO <sub>4</sub>	6.21				3.54				82Sa
		gl	41	0.10	NaClO <sub>4</sub>	6.18				3.42				82Sa
		gl	50	0.10	NaClO <sub>4</sub>	6.10				3.38				82Sa
		ix	25	0.15	NaCl								M+2L=11.10 few details	70B
	La <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.48							pH=7.4	83M
		gl	25	0.10	KCl	6.53	6.53	4.43	4.43	4.02	4.02		pH=8.0, buffer M+2L=10.26, ML+OH=4.04 M+(H <sub>1</sub> L)+OH=11.65	88S
		gl	9	0.10	NaClO <sub>4</sub>	6.07				3.66				82Sa
		gl	17	0.10	NaClO <sub>4</sub>	6.01				3.58				82Sa
		gl	25	0.10	NaClO <sub>4</sub>	5.97	5.97			3.52	3.52			82Sa
														87Sa
		gl	32	0.10	NaClO <sub>4</sub>	5.92				3.45				82Sa
		gl	41	0.10	NaClO <sub>4</sub>	5.88				3.35				82Sa
		gl	50	0.10	NaClO <sub>4</sub>	5.84				3.32				82Sa
	Ce <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.46							pH=8.0, buffer	83M
	Pr <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.51							pH=8.0, buffer	83M
		gl	25	0.10	KCl	6.53	6.53	4.31	4.31	3.76	3.76		M+2L=10.48 ML+OH=4.24 M+(H <sub>1</sub> L)+OH=11.98	88S

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.	
ATP	Nd <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.54						pH=8.0, buffer	83M	
		gl	25	0.10	KCl	6.47	6.47	4.22	4.22	3.60	3.60	M+2L=10.47 ML+OH=4.52 M+(H <sub>1</sub> L)+OH=12.22	88S	
		gl	9	0.10	NaClO <sub>4</sub>	6.40		3.81					82Sa	
		gl	17	0.10	NaClO <sub>4</sub>	6.31		3.67					82Sa	
		gl	25	0.10	NaClO <sub>4</sub>	6.23	6.23	3.63	3.63				82Sa	
		gl	32	0.10	NaClO <sub>4</sub>	6.16		3.57					87Sa	
		gl	41	0.10	NaClO <sub>4</sub>	6.09		3.43					82Sa	
		gl	50	0.10	NaClO <sub>4</sub>	6.00		3.34					82Sa	
Sm <sup>3+</sup>	kin	25	0.05	TAPS.HCl	6.66							pH=8.0, buffer	83M	
	gl	25	0.10	KCl	6.71	6.71	4.51	4.51	3.95	3.95		M+2L=10.53 ML+OH=3.9 M+(H <sub>1</sub> L)+OH=12.28 assume [H] = [Eu]	88S	
Eu <sup>3+</sup>	gl	5	0.20	Me <sub>4</sub> NBr	6.92							pH=6.7 assume [H] = [Eu]	78G	
	gl	15	0.20	Me <sub>4</sub> NBr	7.08							pH=6.7 assume [H] = [Eu]	78G	
	gl	25	0.20	Me <sub>4</sub> NBr	7.26		4.94					pH=6.7 assume [H] = [Eu]	78G	
	gl	35	0.20	Me <sub>4</sub> NBr	7.64							pH=6.7 assume [H] = [Eu]	78G	
	sp	20	0.05	NEM.HCl	6.0							pH=7.0, buffer	74E	
	sp	20	0.05	NEM.HCl	5.9							pH=8.0, buffer	74E	
	kin	25	0.09	PIPES,TAPS	6.8							pH=8.0, buffers	80Ma	
	sp	21	0.10	MES.HCl								ML+L=3.52, buffer pH=6.0	84E	
	kin	25	0.05	TAPS.HCl	6.80							pH=8.0, buffer	83M	
	gl	25	0.10	KCl	6.63	6.63	4.36	4.36	3.75	3.75		M+2L=10.52 ML+OH=4.2 M+(H <sub>1</sub> L)+OH=12.57	88S	
	gl	9	0.10	NaClO <sub>4</sub>	6.48		3.87						82Sa	
	gl	17	0.10	NaClO <sub>4</sub>	6.38		3.75						82Sa	
	Gd <sup>3+</sup>	gl	25	0.10	NaClO <sub>4</sub>	6.31	6.31	3.65	3.65					82Sa
gl		32	0.10	NaClO <sub>4</sub>	6.22		3.58						82Sa	
gl		41	0.10	NaClO <sub>4</sub>	6.16		3.48						82Sa	
gl		50	0.10	NaClO <sub>4</sub>	6.08		3.38						82Sa	
epr		28	0.10	NaCac.	7.0							cacodylate buffer pH=6.0	73V	
kin		25	0.09	PIPES,TAPS	6.0							pH=6.0, buffers	80Ma	
kin		25	0.09	PIPES,TAPS	7.1							pH=8.0, buffers	80Ma	
kin		25	0.09	PIPES,TAPS	6.0							pH=8.7, buffers	80Ma	
kin		25	0.09	PIPES,TAPS	6.0							pH=8.9, buffers	80Ma	
kin		25	0.05	TAPS.HCl	7.06							pH=8.0, buffer	83M	
gl		25	0.10	KCl	6.73	6.73	4.42	4.42	3.88	3.88		M+2L=10.57 ML+OH=4.1 M+(H <sub>1</sub> L)+OH=12.71	88S	
Tb <sup>3+</sup>		kin	25	0.05	TAPS.HCl	7.03							pH=8.0, buffer	83M
		gl	25	0.10	KCl	6.52	6.52	4.17	4.17	3.44	3.44		M+2L=10.39 ML+OH=4.3 M+(H <sub>1</sub> L)+OH=12.95	88S
Dy <sup>3+</sup>	kin	25	0.05	TAPS.HCl	7.31							pH=8.0, buffer	83M	
	gl	25	0.10	KCl	6.44	6.44	4.16	4.16	3.46	3.46		M+2L=10.33 ML+OH=4.4 M+(H <sub>1</sub> L)+OH=13.07	88S	
	gl	9	0.10	NaClO <sub>4</sub>	6.47		3.87						82Sa	
	gl	17	0.10	NaClO <sub>4</sub>	6.43		3.73						82Sa	
	gl	25	0.10	NaClO <sub>4</sub>	6.37	6.37	3.66	3.66					82Sa	
	gl	32	0.10	NaClO <sub>4</sub>	6.32		3.61						87Sa	
	gl	41	0.10	NaClO <sub>4</sub>	6.26		3.53						82Sa	
	gl	50	0.10	NaClO <sub>4</sub>	6.20		3.46						82Sa	
Ho <sup>3+</sup>	kin	25	0.05	TAPS.HCl	7.00							pH=8.0, buffer	83M	
	gl	25	0.10	KCl	6.48	6.48	4.12	4.12	3.39	3.39		M+2L=10.35 ML+OH=4.5 M+(H <sub>1</sub> L)+OH=13.27	88S	



Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria Remarks	Ref.
<u>ATP</u> Er <sup>3+</sup>	kin		25	0.05	TAPS.HCl	7.07						pH=8.0, buffer	83M
	gl		25	0.10	KCl	6.47	6.47	4.04	4.04	3.27	3.27	M+2L=10.47 ML+OH=4.4 M+(H <sub>1</sub> L)+OH=13.54	88S
Tm <sup>3+</sup>	kin		25	0.05	TAPS.HCl	7.42						pH=8.0, buffer	83M
	gl		25	0.10	KCl	6.50	6.50	4.09	4.09	3.47	3.47	M+2L=10.56 ML+OH=4.5 M+(H <sub>1</sub> L)+OH=13.64	88S
	gl		9	0.10	NaClO <sub>4</sub>	6.58			3.90				82Sa
	gl		17	0.10	NaClO <sub>4</sub>	6.51			3.76				82Sa
	gl		25	0.10	NaClO <sub>4</sub>	6.45	6.45	3.67	3.67				82Sa
	gl		32	0.10	NaClO <sub>4</sub>	6.40			3.59				87Sa
	gl		41	0.10	NaClO <sub>4</sub>	6.36			3.49				82Sa
	gl		50	0.10	NaClO <sub>4</sub>	6.28			3.43				82Sa
	kin		25	0.05	TAPS.HCl	7.62							83M
	gl		25	0.10	KCl	6.44	6.44	3.96	3.96	3.20	3.20	pH=8.0, buffer M+2L=10.56 ML+OH=4.6 M+(H <sub>1</sub> L)+OH=13.77	88S
Lu <sup>3+</sup>	kin		25	0.05	TAPS.HCl	7.36						pH=8.0, buffer	83M
	gl		25	0.10	KCl	6.34	6.34	3.88	3.88	3.06	3.06	M+2L=10.47 ML+OH=4.8 M+(H <sub>1</sub> L)+OH=13.68	88S
VO <sup>2+</sup>	kin		25	0.20	KCl	3.72						varies with pH pH=1.5	71K
	kin		25	0.20	KCl	3.97						pH=1.8	71K
	kin		25	0.20	KCl	4.11						pH=2.5	71K
Tl <sup>+</sup> Al <sup>3+</sup>	gl		25	0.15	NaClO <sub>4</sub>	2.0							71M
	kin		25	0.09	?	6.2						pH=7.0	80V
ADP Eu <sup>3+</sup>	gl		25	0.15	NaCl			6.23					87J
	gl		5	0.20	Me <sub>4</sub> NBr	6.76						assume [H] = [Eu] pH=6.7	78G
VO <sup>2+</sup>	gl		15	0.20	Me <sub>4</sub> NBr	6.74						assume [H] = [Eu] pH=6.7	78G
	gl		25	0.20	Me <sub>4</sub> NBr	6.85	4.69					assume [H] = [Eu] pH=6.7	78G
	gl		35	0.20	Me <sub>4</sub> NBr	7.05						assume [H] = [Eu] pH=6.7, buffer	78G
	sp		20	0.05	NEM.HCl	5.75						pH=7.0, buffer	74E
	sp		20	0.05	NEM.HCl	4.89						pH=8.0, buffer	74E
	kin		25	0.20	KCl	3.56						varies with pH pH=1.8	71K
	kin		25	0.20	KCl	3.81						pH=2.6	71K
	gl		25	0.15	NaClO <sub>4</sub>	1.3							71M
	gl		25	0.15	NaCl	10.03						ML-H = -5.85	87J
	AMP-5 Y <sup>3+</sup>	ix		25	0.15	NaCl							M+2L=5.7, pH=7.4, few details
gl			9	0.10	NaClO <sub>4</sub>	4.09			2.56				82Sa
gl			18	0.10	NaClO <sub>4</sub>	4.22			2.78				82Sa
gl			25	0.10	NaClO <sub>4</sub>	4.28			2.78				82Sa
gl			25	0.10	NaClO <sub>4</sub>	4.35	4.35	2.76	2.76				87Sa
gl			33	0.10	NaClO <sub>4</sub>	4.41			2.73				82Sa
gl			41	0.10	NaClO <sub>4</sub>	4.56			2.77				82Sa
gl			50	0.10	NaClO <sub>4</sub>	4.63			2.74				82Sa
gl			9	0.10	NaClO <sub>4</sub>	3.59			2.66				82Sa
gl			18	0.10	NaClO <sub>4</sub>	3.68			2.81				82Sa
gl			25	0.10	NaClO <sub>4</sub>	3.76			2.78				82Sa
gl			25	0.10	NaClO <sub>4</sub>	3.78	3.78	2.76	2.76				87Sa
gl			33	0.10	NaClO <sub>4</sub>	3.84			2.74				82Sa
gl			41	0.10	NaClO <sub>4</sub>	3.91			2.69				82Sa
gl			50	0.10	NaClO <sub>4</sub>	4.02			2.69				82Sa
Nd <sup>3+</sup>	gl		9	0.10	NaClO <sub>4</sub>	3.89			2.83				82Sa
	gl		18	0.10	NaClO <sub>4</sub>	3.99			2.84				82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.05			2.76				82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.09	4.09	2.74	2.74				87Sa
	gl		33	0.10	NaClO <sub>4</sub>	4.16			2.77				82Sa

Table 3. (continued)

Ligand	Metal Ion	Method	T, °C.	Ionic Streng.	Backgr. Electr.	Log K M+L	corr 25°,0.1	Log K M+HL	corr 25°,0.1	Log K M+H <sub>2</sub> L	corr 25°,0.1	Other equilibria	Remarks	Ref.
<b>AMP-5</b>														
Eu <sup>3+</sup>	gl		41	0.10	NaClO <sub>4</sub>	4.26		2.74						82Sa
	gl		50	0.10	NaClO <sub>4</sub>	4.39		2.74						82Sa
	gl		5	0.20	Me <sub>4</sub> NBr	5.72							assume [H] = [Eu] pH=6.7	78G
	gl		15	0.20	Me <sub>4</sub> NBr	5.58							assume [H] = [Eu] pH=6.7	78G
	gl		25	0.20	Me <sub>4</sub> NBr	5.62		3.59					assume [H] = [Eu] pH=6.7	78G
	gl		35	0.20	Me <sub>4</sub> NBr	5.62							assume [H] = [Eu] pH=6.7	78G
	gl		9	0.10	NaClO <sub>4</sub>	4.31		2.70						82Sa
	gl		18	0.10	NaClO <sub>4</sub>	4.42		2.87						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.47		2.74						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.50	4.50	2.72	2.72					87Sa
Dy <sup>3+</sup>	gl		33	0.10	NaClO <sub>4</sub>	4.57		2.80						82Sa
	gl		41	0.10	NaClO <sub>4</sub>	4.67		2.80						82Sa
	gl		50	0.10	NaClO <sub>4</sub>	4.75		2.83						82Sa
	gl		9	0.10	NaClO <sub>4</sub>	4.36		2.76						82Sa
	gl		18	0.10	NaClO <sub>4</sub>	4.46		2.89						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.49		2.73						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.57	4.57	2.71	2.71					87Sa
	gl		33	0.10	NaClO <sub>4</sub>	4.64		2.85						82Sa
	gl		41	0.10	NaClO <sub>4</sub>	4.74		2.86						82Sa
	gl		50	0.10	NaClO <sub>4</sub>	4.83		2.82						82Sa
Tm <sup>3+</sup>	gl		9	0.10	NaClO <sub>4</sub>	4.32		2.52						82Sa
	gl		18	0.10	NaClO <sub>4</sub>	4.37		2.86						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.46		2.72						82Sa
	gl		25	0.10	NaClO <sub>4</sub>	4.46	4.46	2.70	2.70					87Sa
	gl		33	0.10	NaClO <sub>4</sub>	4.55		2.70						82Sa
	gl		41	0.10	NaClO <sub>4</sub>	4.64		2.72						82Sa
(CH <sub>3</sub> ) <sub>3</sub> Sn <sup>+</sup>	gl		50	0.10	NaClO <sub>4</sub>	4.82		2.62						82Sa
	gl		25	0.30	NaClO <sub>4</sub>	3.31		1.59					ML+L = 1.42	87H
<b>IMP-5</b>														
(CH <sub>3</sub> ) <sub>3</sub> Sn <sup>+</sup>	gl		25	0.30	NaClO <sub>4</sub>	2.52							ML+M = 2.85	87H
<b>TMP-5</b>														
Fe <sup>3+</sup>	red		20	0.10	NaClO <sub>4</sub>	8.60							ML-H = -2.59	68R

Method: cal = calorimetric, epr = electron paramagnetic resonance, gl = potentiometric using glass electrode, int = interferometric, ise = potentiometric using ion selective electrode, ix = ion exchange, kin = kinetic, lit = literature survey, nmr = nuclear magnetic resonance, red = potentiometry using redox electrode, sp = spectrophotometric, ? = not given in paper.

#### IV. DISCUSSION OF CONSTANTS

##### Enthalpy Changes Accompanying Complexation

Before evaluating complexation constants, it was necessary to make a critical evaluation of the enthalpy changes that accompany complexation in order to correct reported constants to 25°C so that direct comparisons may be made.

The reported enthalpy values are listed in Table 1. The units kJ/mol are employed. These may be converted to kcal/mol by dividing the values by 4.184. The final recommended values are listed in Table 4 with an estimate of the uncertainty for each value.

Batch calorimetry, in which the metal ion solution and the ligand solution are rapidly combined and the heat change measured directly, is the most reliable and precise method for obtaining enthalpy changes but results from this method are not available for all complexes. Titration calorimetry, in which heat change is measured as increments of solution are added, is less precise and has greater chance of misinterpretation of results but usually gives satisfactory values. Enthalpy changes can also be calculated from complexation constants measured at several temperatures. If the complexation constants are measured carefully in cells without liquid junction potentials, at small temperature intervals over a large temperature range, with consideration of heat capacity changes, the precision is similar to that from titration calorimetry. However with junction potentials and fewer temperature measurements the precision is much less and at best gives only an order of magnitude. At worst it gives completely misleading results. Therefore temperature variation of potentiometric data involving liquid junction potentials were selected cautiously only when no other values were available. In a few cases, the enthalpy change was calculated from data in the paper although the authors did not report a value.

##### Protonation Enthalpy Changes

For the first protonation of ATP, two of the calorimetric results agree closely but the third is considerably more exothermic than the others. The agreement of the first two is apparently fortuitous since their ADP, AMP-5, and second protonations do not show this agreement. In reference 62C, results for the first protonation of triphosphate (TP) and diphosphate (DP) are also considerably more endothermic than two other calorimetric results with each ligand. In addition, the two more exothermic results for TP (65A: -0.4 kJ/mol at 0.1 ionic strength, 66I: -0.4 at 0.65 ionic strength) are almost identical with the more exothermic result with ATP (-0.8 kJ/mol) as would be expected if the first protonation involves the triphosphate portion of ATP. Protonation at the triphosphate moiety would be expected, rather than at the adenosine moiety, because the protonation constant of ATP (6.53) is much closer to that of TP (7.97) than to that of adenosine (3.55). Therefore the value of 81C (-0.8 kJ/mol), supported by the less accurate temperature variation values of 51A, 66T, and 86D, is recommended for the first protonation constant of ATP. The difference between the 81C and 87Sa values is about the same as the difference in the second protonation constants which suggests that 87Sa has a calibration error. There are insufficient data to determine the effect of ionic strength and background electrolyte on the enthalpy value. The available data suggest that the effect of these variables is less than the estimated uncertainty of the measurements from zero to 0.2 M ionic strength and perhaps beyond.

The second protonation enthalpy values of 81C and 62C at zero ionic strength are in excellent agreement and in close agreement with the calorimetric protonation enthalpy value of adenosine (70C: -16.3 kJ/mol at near zero ionic strength and 60R: -15.9 kJ/mol at 0.1 M ionic strength). The recommended value for adding the second proton to ATP is that of 81C (-15.1 kJ/mol) supported by 62C, 66T, 80Tb, and 86D. The sign and magnitude of the enthalpy values show that the second proton coordinates to the purine ring rather than the triphosphate group.

The other nucleotide triphosphates, GTP, ITP, CTP, and UTP, have only been reported in two papers in which the temperature variation method was employed. There is no agreement for the first protonation enthalpy value. The value of 65P shows only a small change from its ATP value which is what would be expected if the first proton coordinates to the triphosphate and therefore 65P is probably the more reliable. However the magnitude for the ATP value is somewhat different from the recommended value and suggests an experimental error. If the suspected error is common to all of the measurements, such as a change in junction potential with temperature, then the relative values could still be accurate because of error cancellation upon subtraction. Therefore tentative values for the first protonation enthalpies were obtained by adjusting the values of 65P so that the value for ATP agrees with the recommended value for ATP selected above.

The first protonation enthalpy values for the corresponding mono- and diphosphates were evaluated in the same way as the triphosphates based on the values of 65P relative to the recommended value of ATP and are tentatively recommended.

The enthalpy values of 73T and 83R for the second protonation of the nucleotide triphosphates are near the values for ATP and are probably approximately correct since the second proton would be expected to involve a ring nitrogen as with ATP. Calorimetric values for guanosine (70C: -13.4 kJ/mol at near zero ionic strength and 60R: -4.2 at 0.1 M ionic strength) suggest a value near -13 kJ/mol instead of the -17 value of 73T for GTP and for cytosine (67C: -21.3 kJ/mol at near zero ionic strength and 60R: -18.8 kJ/mol at 0.1 M ionic strength) suggest a value near -21 kJ/mol instead of the -17 value for CTP. Therefore the uncertainty of the measurements appears to be at least four kJ/mol and perhaps slightly more.

The second protonation enthalpy values of adenosine and its phosphate derivatives determined calorimetrically are all about the same (-16 ± 1 kJ/mol) and the less precise values with cytosine and its phosphate derivatives are also in agreement (-20 ± 4 kJ/mol). Therefore the other nucleotides should not vary

more than  $\pm 4$  kJ/mol as the number of phosphates changes. Estimates based on the 73T and 83R values are tentatively recommended for adding the second proton to the mono-, di-, and triphosphates.

The enthalpy value for the first protonation of ADP cannot be based upon 62C or 87Sa since those papers reported values which were too endothermic for ATP. The temperature variation values do not show good agreement but the differences between the ATP and the ADP enthalpies of each paper that measured both values show much better agreement. If the zero ionic strength value of 62C and the value of 80T are omitted, the ADP enthalpy is  $-2.1 \pm 0.8$  kJ/mol relative to the ATP value for the eight other comparisons. Therefore the ATP value adjusted by this amount to  $-2.9$  kJ/mol is recommended for adding the first proton to ADP.

For the second protonation of ADP, the differences between the ATP and ADP values for 51A, 66T-67T, and 78G adjusted to the ATP value are in good agreement with the zero ionic strength value of 62C and since the 62C value for ATP is in excellent agreement with the recommended value for that ligand, its value ( $-17.2$  kJ/mol) is recommended for adding the second proton to ADP.

The average of seven out of ten differences between the first protonation enthalpy values for AMP-5 and those for ADP is  $2 \pm 1$  kJ/mol. Therefore the ADP value adjusted by this amount to  $-4.2$  kJ/mol is recommended for adding the first proton to AMP-5.

The calorimetric value of 62C for zero ionic strength ( $-17.6$  kJ/mol), supported by 74B and 88A and by the differences from ADP of 51A, 67T, and 80T, is recommended for the second protonation enthalpy of AMP-5.

The values of 67T, adjusted relative to the AMP-5 value, are tentatively recommended for the protonation enthalpy values of AMP-3 and AMP-2. The 51A value for AMP-3 is in approximate agreement.

The few enthalpy values reported for the third and fourth protonations of the nucleotides are not recommended.

#### Alkali Metal Complex Enthalpy Changes

The calorimetric results of 81C, supported by 86D, are tentatively recommended for the enthalpy changes accompanying the formation of the  $\text{Na}^+$  and  $\text{K}^+$  complexes with ATP at  $-0.8$  and  $+1.3$  kJ/mol. The temperature variation results of 86D for  $\text{Li}^+$ ,  $\text{Rb}^+$ , and  $\text{Cs}^+$  are tentatively recommended after rounding to the nearest kJ/mol because of the expected lower precision. The reported enthalpy changes for the complexation of the alkali metal ions with mono-protonated ATP to form MHATP and of  $\text{Li}^+$  with LiATP to form  $\text{Li}_2\text{ATP}$  are not recommended. They depend upon minor variation of approximate values and may be completely in error.

#### Alkaline Earth Metal Complex Enthalpy Changes

The calorimetric results of 69B and 82S from the same research group show the variation of the enthalpy change of  $\text{Mg}^{2+} + \text{ATP}$  with temperature. A linear extrapolation to  $25^\circ\text{C}$  indicates  $+19.01$  kJ/mol which is in approximate agreement with the results of 87Sa ( $+18.07$ ). When the 87Sa value is corrected for the background electrolyte using the NaATP value ( $-0.8$ ), the result ( $+18.8$ ) is in excellent agreement and  $+18.8$  kJ/mol is recommended for MgATP. The temperature variation results of 57N, 59B, 66P, 66T (when the  $40^\circ\text{C}$  value is omitted), 71B, and 73B show good agreement. This value is also supported by the results of 65A for  $\text{Mg}^{2+}$  with TP ( $+18.0$  kJ/mol).

For  $\text{Mg}^{2+} + \text{HATP}$ , the calorimetric results of 87Sa, rounded to  $+9.6$  and supported by 66P and 66T (when the  $0^\circ\text{C}$  value is omitted), is recommended.

The calorimetric value of 87Sa, corrected for the background electrolyte to  $+14.2$  kJ/mol, is recommended for  $\text{Ca}^{2+} + \text{ATP}$ . The temperature variation result of 57N is in approximate agreement. For the CaTP complex, the calorimetric results of 65A and 77R show very good agreement at  $+13.8$  kJ/mol which strongly suggests that the CaATP complex should be similar unless the  $\text{Ca}^{2+}$  is not complexed to the triphosphate portion. It would be expected that the triphosphate group would be a stronger coordinator for  $\text{Ca}^{2+}$  than the adenosine portion as indicated by the stability constant trend of  $\text{Ca}^{2+}$  with TP (6.35)(65A), ATP (4.25), ADP (3.08), and AMP-5 (1.80). If CaATP has the same relationship to CaTP as MgATP has to MgTP then the enthalpy change for the formation of CaATP should be about  $+14.6$  kJ/mol and supports the value of 87Sa recommended above ( $+14.2$ ).

For CaHATP, the value of 87Sa rounded to  $+7.9$  kJ/mol is tentatively recommended. The values for  $\text{CaH}_2\text{ATP}$  and  $\text{Ca}_2\text{ATP}$  by 86D are not recommended.

The endothermic value of  $\text{Sr}^{2+}$  with TP (72S) suggests that the reported  $\text{Sr}^{2+}$  and  $\text{Ba}^{2+}$  values with ATP are in error and are not recommended. The less certain MHL values are not recommended.

The calorimetric results of 73S for  $\text{Mg}^{2+}$  with GTP, ITP, and UTP show only small variations from that of ATP as would be expected from the similarity of the primary coordinating group and are tentatively recommended. The temperature variation results of 73T are too uncertain to be of any value. The results of 83R with CTP and with UTP do not agree with the other triphosphates and are not recommended.

The two calorimetric results for  $\text{Mg}^{2+}$  with ADP reported by 69B and 87Sa are in considerable disagreement. The trends from ATP to ADP to AMP-5 for protonation, for transition metal complexes, and for 73S with  $\text{Mg}^{2+} + \text{guanosine}$  and  $\text{uridine}$  phosphates are in uniform steps to more exothermic values as the number of phosphates decreases. This supports the 69B trend and puts doubt on the 87Sa value. Therefore the 69B value at  $+13.4$  kJ/mol, supported by the temperature variation values of 66P and 67T, is recommended for MgADP.

The MgHADP value of 87Sa at +7.5 kJ/mol is tentatively recommended. The temperature variation value of 66P is in approximate agreement.

The  $\text{Ca}^{2+} + \text{ADP}$  value of 87Sa seems much too endothermic relative to the CaATP and CaAMP-5 values in the same paper and is not recommended.

The CaHADP value of 87Sa is the approximate magnitude that would be expected by the trend from CaHATP and is tentatively recommended.

The calorimetric values of 87Sa for CaAMP-5 is also tentatively recommended. The  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  values for complexes with ADP, AMP-3, AMP-2 of 67T are not recommended.

The calorimetric values of 73S for  $\text{Mg}^{2+}$  with GDP, UDP, GMP-5, and UMP-5 are tentatively recommended.

For  $\text{Mg}^{2+}$  with AMP-5, the two calorimetric results are in approximate agreement, but for consistency with the other recommended values, +7.5 kJ/mol from 69B is tentatively recommended.

The CaAMP-5 value of 87Sa at +4.2 kJ/mol is tentatively recommended.

The values of 67T for  $\text{Mg}^{2+}$  with AMP-3 and with AMP-2, after they are adjusted by the same amount as is necessary to change the MgAMP-5 value in the same paper to the recommended MgAMP-5 value, are tentatively recommended at +7.9 kJ/mol.

#### Transition Metal Complex Enthalpy Changes

The calorimetric values of 77R, 78G, and 83A are tentatively recommended for the complexation of  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cu}^{2+}$ , and  $\text{Zn}^{2+}$  with ATP. For  $\text{Mn}^{2+}$  with ATP, a 25°C value was estimated by assuming a linear change between the 15° and 30° values. The value for  $\text{Ni}^{2+}$  with ATP was estimated by comparing the Mn to Co to Cu trend with ATP to the Mn to Co to Ni trend with ADP.

The enthalpy changes for the transition metals with the other nucleotide triphosphates would be expected to be similar to those with ATP and therefore the highly uncertain temperature variation values of 73T, 76T, and 83R are not recommended.

With ADP and with AMP-5, the calorimetric values of 77R and 79M are tentatively recommended for the  $\text{Mn}^{2+}$  and  $\text{Ni}^{2+}$  complexes. With  $\text{Co}^{2+}$ , the temperature variation values of 80M seem to fit the observed trend and are tentatively recommended. Estimates of  $\text{Cu}^{2+}$  and of  $\text{Zn}^{2+}$  values were made by comparison to the Mn to Zn trend with ATP.

The temperature variation values of 67T for AMP-3 and for AMP-2, adjusted in the same manner as the variation between their AMP-5 values and the recommended AMP-5 values, are tentatively recommended. The values of 88A for CuAMP-5 appear to be too exothermic, the experimental uncertainty is rather large, and they are not recommended.

#### Other Metal Complex Enthalpy Changes

The temperature variation values of 78G and of 87Sb for  $\text{Eu}^{3+} + \text{ATP}$  and AMP-5 are in complete disagreement. The trend of 78G from EuATP to EuAMP-5 is much more similar to the trend with protonation and metal complex enthalpy changes with these ligands than is the trend of 87Sb. Therefore the results of 78G for EuATP, EuADP, and EuAMP-5, rounded to the nearest kilojoule, are tentatively recommended. The value with ADP fits the trend from ATP to ADP to AMP-5 better, in comparison to the complexes of  $\text{Mg}^{2+}$  with the same ligands, if the 5°C value is omitted and a linear trend is assumed for the other temperatures.

#### Protonation Constants

##### ATP

The reported log *K*'s for adding the first proton to ATP, listed in Table 2, range from 7.70 to 5.47 but when ionic strength, temperature, and the cation of the background electrolyte are taken into consideration, the majority of values are in good agreement. Consequently the values in the table are grouped firstly according to the cation of the background electrolyte and secondly according to ionic strength.

Mixed protonation constants (also known as Bronsted or as practical constants), involving both hydrogen ion activity and ligand concentration terms, were converted to concentration constants by using hydrogen ion activity coefficients. Usually the conversion was necessary at 0.1 to 0.2 ionic strength where the activity coefficient is essentially independent of the background electrolyte and 0.78 was used. After correction, the logarithm of the mixed constant is 0.11 lower. In some papers it was not clear which type of constant was calculated. Comparison of the reported values with those known to be concentration constants frequently gave an indication of the type of constant reported.

The zero ionic strength value of 63P appears to be accurately measured and is tentatively recommended. The calculated value of 86D, based on measurements at higher ionic strength, is in very good agreement but the calculated value of 80Ta does not agree and probably involves a computational error.

The reported values for the first protonation constant near 0.1 M ionic strength were converted to 25°C by using the  $\Delta H$  value selected in this paper, to 0.10 M ionic strength by using the observed changes with ionic strength of 63P and 86D, and to concentration constants (76S), and the new value listed in the next column of the table. The values at 0.10 M ionic strength were selected for each background electrolyte and the average of the majority that showed good agreement are listed in Table 5. Minority values with poor agreement are assumed to involve some unknown experimental or computational error. The 81C value in  $\text{Et}_4\text{NBr}$  was not used even though their values for the second protonation constant and those in  $\text{KNO}_3$  and in  $\text{NaClO}_4$  were used because it does not agree with the mutually consistent values of 54M, 56S, 63Pa, and 64O. The values of 73Sa, 77R, and 78G are in good agreement with each other but are from the same research group. They are

higher than what would be expected based on the majority of other values and 78G is also larger than the majority for the second protonation constant. Therefore their values were not used in the selection of the recommended constants.

There is a decreasing magnitude of the recommended values for the first protonation constant of ATP from that in  $\text{Pr}_4\text{N}^+$  (6.96 from 56S, 63P, and 86D) to  $\text{Et}_4\text{N}^+$  (6.93 from 54M, 56S, 64O, 86D, and 87Sa) to  $\text{Me}_4\text{N}^+$  (6.79 from 56S, 66Pa, and 86D) to  $\text{K}^+$  (6.50 from 56M, 56S, 62T, 72F, 81C, and 86D) to  $\text{Na}^+$  (6.44 from 51A, 56B, 56S, 64Sa, 71M, 78R, 80Tb, 81C, 83J, 83W, 84Sa, 85T, 86D, 87S, 87Sa, and 87Sc). This progression suggests NaATP and KATP complexes which compete with the protonation and perhaps also  $\text{Me}_4\text{NATP}$  and  $\text{Et}_4\text{NATP}$  complexes as suggested by 85D and 86D. However a more likely explanation of the latter trend is that as the background electrolyte changes to larger, more hydrophobic groups, the hydration layers around the ions are decreased, there is less disruption upon adding a proton, and the solvent becomes more non-aqueous in nature.

The recommended value for biological conditions (37°C and 0.15 M ionic strength with sodium ions) was calculated from the recommended value at 25°C and 0.10 M sodium ions, the enthalpy change, and the expected change with a change of ionic strength. Values for the first protonation constant in other background electrolytes can be estimated by subtracting 0.04 from the recommended value at 25°C and 0.10 M ionic strength.

For values at higher ionic strength, the trends of 86D in tetraalkylammonium salts are probably only valid in the specific background electrolyte and the increasing trend above 0.25 M  $\text{Pr}_4\text{N}^+$ , 0.25 M  $\text{Et}_4\text{N}^+$ , and 0.49 M  $\text{Me}_4\text{N}^+$  is perhaps dominated by the increasing non-aqueous nature of the solvent. The trends with ionic strength in  $\text{K}^+$  or  $\text{Na}^+$  salts are almost identical, which would be expected if the charge of the reactants is the predominant factor. The trend of 54M from 0.15 to 0.3 M  $\text{Et}_4\text{N}^+$  and the value of 76R in 1.00 M  $\text{K}^+$  are in agreement with the values of 86D, adjusted in the same manner as the differences between their 0.10 M value and the recommended 0.10 M values, but the trends of 79Mb and of 80Tb in  $\text{Na}^+$  media do not agree with 86D or each other. The values of 86D to 1.00 M ionic strength, after adjusting to the recommended 0.10 M values, are tentatively recommended.

The second protonation values of ATP seem to be independent of the background electrolyte at about 4.00. This would be expected since the sign and magnitude of the enthalpy change are consistent with nitrogen bonding and nitrogen would be expected to have no or extremely weak  $\text{Na}^+$  or  $\text{K}^+$  bonding. The value under biological conditions would be expected to be about 3.88.

Adding a second proton at higher ionic strength seems to indicate an independence of background electrolyte for 0.25 M and for  $\text{Na}^+$  and  $\text{K}^+$  media through 1.00 M ionic strength. Values based on 86D, 76R(K), 80Tb(Na), and 79Mb(Na, 0.5 M) are recommended in Table 5. The values are compatible with a small increase from 0.25 to 1.00 M ionic strength which would be expected with nitrogen bonding. The values in  $\text{Pr}_4\text{N}^+$  media show a larger increase with ionic strength which may indicate an additional non-aqueous effect and are tentatively recommended. The values in  $\text{Et}_4\text{N}^+$  and in  $\text{Me}_4\text{N}^+$  media show a decrease which is not expected and they are not recommended.

The value of 83S of 1.91 for adding the third proton to ATP at zero ionic strength is tentatively recommended. The average value of 79Mb, 88B and 88T after rounding to 1.8 because of expected lower accuracy is recommended for 0.10 M ionic strength.

### AQP

The protonation constants for AQP have been reported at 20°C or at 0.20 M ionic strength and no direct information is available for the enthalpy change or the change with ionic strength. Based on the trend from AMP-5 to ADP to ATP, the enthalpy change for AQP is estimated as +1.7 kJ/mol for the first protonation and -13.0 kJ/mol for the second protonation; while the change of  $\log K$  with 0.10 M change in ionic strength is estimated as 0.15 for the first protonation and 0.07 for the second protonation for values near 0.1 M ionic strength. These values were used to convert the reported values to 25°C and 0.10 M ionic strength. The two reported values have good agreement for a potassium ion background at 6.77 which is recommended for the first protonation constant of AQP. The tentatively recommended constants for other background electrolytes are based on that average and the differences between values measured in different background electrolytes by 56S. The adjusted second protonation constant of 57S at 4.05 is also tentatively recommended. This is almost the same as that for ATP which is expected because the second proton involves the adenosine portion of the molecule.

### Other Nucleotide Triphosphates

For the other nucleotide triphosphates, there are only a few values and evaluation must be made on isolated values or between disparate values. Values from 65P show that the triphosphates are almost identical for the first protonations at zero ionic strength and strongly indicates that they should be almost identical under other conditions. Therefore ATP values were used as a guide to recommend 65P values for zero ionic strength and with a tetrapropylammonium ion background with GTP, ITP, CTP, and UTP; the average of 56B and 77S for GTP with a sodium ion background; the average of 77S and 77Sa for ITP with sodium ions; the average of 72F and 84M for CTP with potassium ions; the average of 77S, 84Sa, and 87S for CTP with sodium ions; the average of 77S, 85T, and 87S for UTP with sodium ions; and 77S and 87S for TTP with sodium ions.

The second protonation values for the other nucleotide triphosphates would be different from those of ATP because of the involvement of a different nitrogen base but comparisons may be made with the

corresponding diphosphates and monophosphates after adjusting the values to correspond to the differences between ATP and ADP and AMP. The values of 73T for GTP and ITP, of 84Sa for CTP, and of 85T for UTP are tentatively recommended.

The loss of a proton at high pH has been reported for GTP, ITP, and UTP. The log protonation constants of 75S at 9.68, 9.15, and 9.59 are tentatively recommended for GTP, ITP, and UTP. The value of 83R for UTP is completely different from the other values and is not recommended.

#### ADP

The recommended protonation constants of ADP were selected in a manner similar to the selection of the ATP constants. The values of 6.65 in  $\text{Pr}_4\text{N}^+$  (based on 56S and 63P), 6.63 in  $\text{Et}_4\text{N}^+$  (based on 54M, 56S, and 64O), 6.55 in  $\text{Me}_4\text{N}^+$  (based on 56S, 77R, and 78G), 6.36 in  $\text{K}^+$  (based on 56M, 56S, 72F, and 80D) and 6.31 in  $\text{Na}^+$  (based on 56B, 56S, 71M, 75K, and 87Sa) are recommended. At 37°C and 0.15 M, this becomes 6.27 in the presence of sodium ion.

For adding a second proton to ADP, the value 3.94 based on 56M, 62Ta, 72F, and 87Sa is recommended. At 37°C and 0.15M, this constant becomes 3.82. The second protonation value of 78G is considerably higher than the other values as it is with ATP and so its second, third, and fourth protonation values are not recommended.

#### Other Nucleotide Diphosphates

The other nucleotide diphosphate protonation constants were selected in the same way as were the triphosphate values. The values of 65P for the first protonation of GDP, IDP, CDP, and UDP for zero ionic strength and in tetrapropylammonium ion background, of 56B for the first and second protonations of GDP, of 56B( $\text{Na}^+$ ) and 72F( $\text{K}^+$ ) for the first protonation of CDP, of 72F and 73B(same research group as 72F) for the second protonation of CDP, and of 56B for the first protonation of UDP are tentatively recommended. The 56B values for the loss of a proton at high pH were not recommended with the triphosphates and are not recommended for GDP and UDP.

#### AMP

With AMP-5, the recommended protonation constants were selected in much the same manner as that employed for ATP and for ADP. The values of 6.67 at zero ionic strength from 63P; of 6.35 in 0.10 M  $\text{Pr}_4\text{N}^+$  from 56S and 63P; of 6.34 in 0.10 M  $\text{Et}_4\text{N}^+$  from 56S; of 6.29 in 0.10 M  $\text{Me}_4\text{N}^+$  from 56S, 61T, 77R, and 78G; of 6.21 in 0.10 M  $\text{K}^+$  from 56S, 61T, 62T, 72F, 74B, 75B, and 88A; and of 6.18 in 0.10 M  $\text{Na}^+$  from 56S, 76Ta, 79T, 87T, and 88Sa were selected for adding the first proton to AMP-5. For biological conditions this becomes 6.14. Adding the second proton appears to be independent of background electrolyte with a value of 3.80 from 56M, 62Ta, 66R, 72F, 74B, 75B, 76O, 76T, 78G, 80O, 80Tb, 87T, 88A, and 88Sa, and becomes 3.67 at 37°C and 0.15 M ionic strength. The values of 78G for the first and second protonation constants show excellent agreement with the other values in contrast to ATP and ADP but their value for the third protonation constant seems to be too large and is not recommended.

For AMP-3, the value of 5.80 from the average of 62Ta and 80Ta in potassium ion media and 5.72 from the average of 51A, 76Ta, 87T and 89M in sodium ion media are recommended. Adding the second proton has the value 3.60 based upon 51A, 62Ta, 76O, 76Ta, 87T, and 89M.

For AMP-2, the median of values from 67T, 72F, and 80Ta at 6.01 and 3.70 for the first and second protonations in potassium ion media are recommended. The average values of 87T and 89M from the same research group at 5.85 and 3.64 are tentatively recommended for sodium ion media.

#### Other Nucleotide Monophosphates

The values of 65P for adding the first proton to GMP-5, to IMP-5, to CMP-5, and to UMP-5 at zero ionic strength and in tetrapropylammonium ion background; of 79T, 83C, and 88Ma to GMP-5 in sodium ion media; of 58Wa, 72F, 80O, 84M, and 85K to CMP-5 in potassium ion media; of 56B and 88M to CMP-5 in sodium ion media; and of 84S and 88M to UMP-5 in sodium ion media are all recommended. Values for adding the second proton to GMP-5 by 56B, 76O, and 88Ma; to GMP-3 by 76O; to CMP-5 by 56B, 58Wa, 70W, 72F, 76O, 79T, 80O, 85K, and 88M; to CMP-3 by 76O; and to TMP-5 by 88M are also recommended. The values for removing a proton at high pH by 56B, 63S, and 83C with GMP-5, 81N and 87H with IMP-5, and 68R with TMP-5 are not recommended. The average of 56B, 63S, 67A, 76O, and 88M at  $9.39 \pm 0.05$  for UMP-5 is recommended and the value of 88M at 9.79 for TMP-5 is tentatively recommended.

The recommended protonation constants are collected in Table 5 with an estimate of the uncertainty for each value.

#### Alkali Metal Constants

In addition to the reported log  $K$  values for alkali metal complexes in Table 3, there are values calculated from the change of protonation constants as the media is changed from tetramethylammonium ion to potassium ion or to sodium ion. Since the protonation constants have been measured more often and can be measured with greater accuracy than the alkali metal constants, these values should be more accurate for the conditions of measurement, i.e., 25°C and 0.10 molar in alkali metal ion concentration. They were calculated from the expression:

$$\text{Log } K(\text{H}^+ \text{ in } \text{Me}_4\text{N}^+) - \text{Log } K(\text{H}^+ \text{ in } \text{K}^+ \text{ or } \text{Na}^+) = \text{Log}(1 + 0.10 K_{\text{ML}}).$$

The order of magnitude of stability constants for the alkali metal complexes from the majority of workers is:  $\text{Li}^+ > \text{Na}^+ > \text{K}^+ > \text{Rb}^+ > \text{Cs}^+$  as would be expected from ion size. However a few (54M, 59W, 64O, 70M, 76K) report very little or no difference between sodium ion and potassium ion values.

Constants calculated from protonation constants in the two media agree with the majority and show a significant difference between  $\text{Na}^+$  and  $\text{K}^+$  values.

The  $\text{Li}^+$ ,  $\text{Na}^+$ , and  $\text{K}^+$  complexes with AQP have been measured only by 56S and show a relatively large difference between the alkali metal constants as would be expected from the large charge on the ligand. The values in  $\text{Me}_4\text{N}^+$  are not given in the paper but were calculated from their data (in Table I of 56S) and by use of the above equation (with 0.20 instead of 0.10). The constants were measured with a large excess of alkali metal ions and since it was shown by 62T that the use of an excess of  $\text{Mg}^{2+}$  lowers the magnesium stability constant with ATP, it is concluded that these constants are probably low. Using the same correction (0.22) as discussed and used with ATP and with ADP below, the values of 2.22 for  $\text{Li}^+$ , 1.71 for  $\text{Na}^+$ , and 1.54 for  $\text{K}^+$  are tentatively recommended for AQP in 0.10 M  $\text{Me}_4\text{N}^+$  media.

The  $\text{Na}^+$  complex with ATP is the most studied of the alkali metal constants. The reported values range from 2.36 at zero ionic strength to 0.80 at 0.20 M ionic strength. The work of 56S and that of 86D show a dependence upon the background electrolyte which suggests that the values need to be adjusted to the same background electrolyte for comparison. Tetramethylammonium ion seems to be the logical choice because of its less hydrophobic nature. After adjusting to tetramethylammonium ion media by the use of the relative values of 56S and to 0.10 M ionic strength as with the protonation constants, a trend is apparent from 0.75 (54M at 0.30 M ionic strength) to 0.87 (56S at 0.20 M ionic strength) to 1.10 (from average of protonation values at 0.10 M ionic strength). This suggests that correction can be made for the excess sodium ions by extrapolating to 0.00 M ionic strength. The difference between the 0.10 M values from the average of the protonation constants to 0.20 M values is 0.23 for 56S with sodium ions, 0.25 with potassium ions, 0.22 for 54M with sodium ions, and 0.19 with potassium ions, for an average of 0.22. Adjusting the value from protonation constants by this amount gives 1.32 which agrees with 1.33 from 81C, 1.29 from 65B and 1.29 from 87Sa. The result of 64O, where 0.02 M N-ethylmorpholine and 0.08 M NaCl were used, also agrees at a value of 1.34 if it is assumed that N-ethylmorpholine has half the effect of tetraethylammonium ion because it is intermediate between tetraethylammonium and tetramethylammonium in the number of carbon atoms. The value of 56S becomes 1.31 and that of 54M becomes 1.32 after adjusting for the excess sodium ion. The values of 78A at 1.45 and 70M at 1.56 are considerably higher. The value of 86D at 1.37 is based on tetrapropylammonium ion rather than tetramethylammonium ion media and if the differences between the protonation values of these two ions is used, the constant corrects to 1.26, which is somewhat lower than the other values. The average of the majority of the reported constants, 1.31, is recommended for the  $\text{Na}^+$  complex with ATP in 0.10 M tetramethylammonium ion media, which is adjusted to 0.95 at 37°C and 0.15 M sodium ion media.

The MHL values of  $\text{Na}^+$  with HATP as well as those for the other alkali metal ions reported by 86D are insignificant as would be expected from nitrogen coordination. Since such small values cannot be measured accurately by the potentiometric method, these constants are not recommended.

The values of the  $\text{K}^+$  complex of ATP treated as with the  $\text{Na}^+$  complex gives adjusted values of 1.15 for 81C, 1.15 for 86D, 1.16 for 65B, 1.17 from the protonation constants, 1.20 for 56S, 1.25 for 54M, 1.27 for 64O, 1.41 for 70B, and 1.54 for 70M. Since 54M, 64O, and 70M have almost identical values for the sodium and potassium ion complexes, contrary to the results of the majority of the workers, the lower values would be preferred and the average of 1.17 is recommended for 0.10 M tetramethylammonium ion media and 0.81 at 37°C and 0.15 M sodium ion media.

Since the values of 65B for the sodium and potassium complexes agree with the recommended values, their  $\text{Rb}^+$  and  $\text{Cs}^+$  values at 1.11 and 1.06 are tentatively recommended for tetramethylammonium media. The values of 86D for these ions do not fit the expected trend based on ionic size.

The value of 1.78, with greater uncertainty than with the sodium and potassium values, is recommended for the  $\text{Li}^+$  complex with ATP in 0.10 M tetramethylammonium media. This is the average of the 56S value adjusted to 1.86 as above, the adjusted 86D value (1.73), and the 65B value (1.73).

With ADP, the average difference between the 0.10 M values for NaADP and KADP from the protonation constants and those of 54M and 56S at 0.20 M adjusted to 0.10 M is 0.22 which is the same as with ATP. By the use of an adjustment for excess alkali metal ions as with ATP, the adjusted values for NaADP are 0.8 for 78A, 1.07 for 54M, 1.10 for 56S, and 1.14 for the value from the protonation constants. Since the values of 54M show  $\text{KADP} > \text{NaADP}$ , the average of the two largest values at 1.12 is recommended for the complex of  $\text{Na}^+$  with ADP in 0.10 M tetramethylammonium media.

Treating the values for the  $\text{K}^+$  complex with ADP in the same way as NaADP gives adjusted values of 0.99 from the protonation constants, 0.99 from 70B, 1.01 from 56S, 1.09 from 54M, and 1.56 from 74F. The average of the lower three at 1.00 M is recommended for the  $\text{K}^+$  complex with ADP in 0.10 M tetramethylammonium media.

The adjusted value of 56S at 1.32 is tentatively recommended for the complex of  $\text{Li}^+$  with ADP in 0.10 M tetramethylammonium media.

The difference between the 56S values and those from the protonation constants for NaAMP-5 and KAMP-5 is 0.35. Use of this value to adjust for excess alkali metal ion gives values of 0.48 for 61T, 0.87 for 56S, 0.88 from the protonation constants, and 1.5 for 76K. The value of 0.88 is recommended for the  $\text{Na}^+$  complex with AMP-5.

A similar adjustment for the potassium complex gives 0.70 from the protonation constants, 0.72 for 56S, 0.98 for 70B, and 1.5 for 76K. The value recommended for the  $\text{K}^+$  complex with AMP-5 is 0.70.



The adjusted value of 56S to 1.22 is tentatively recommended for the complex of  $\text{Li}^+$  with AMP-5.

The alkali metal complexes of the other nucleotides have not been measured but since they likely involve only the phosphate portion of the molecule as with the adenosine phosphates, the constants are probably very similar to those of the corresponding adenosine-5'-phosphates.

### Alkaline Earth Metal Complexation Constants

#### Magnesium Complexes of ATP

The formation constant of  $\text{Mg}^{2+}$  with ATP has been measured many times with rather discordant results. About fifty papers have reported values which range from 5.35 to 3.62 after being converted to 25°C, 0.10 M ionic strength, and after correction for sodium or potassium complex formation.

The potentiometric results of 84G are higher than all other values but the protonation constant reported by that paper is about 0.5 units higher than the recommended value and if the recommended value had been used in the calculation, the magnesium constant would be much lower. Similarly the protonation constant of 79Mc is about 0.1 units too large and recalculation would give a lower value.

The high results of 70B were corrected for chloride ion by the use of an unpublished complexation value for  $\text{MgCl}_2$  which is about 0.3 units larger than published values (see 89S). Here the use of the proper chloride complexation constant would produce a lower value.

The results of 74M are high because of the use of a large constant for the sodium complex with ATP to correct for sodium ions present in the measured solutions. A plot of the formation constant against sodium ion concentration from Table I of that paper shows a definite trend. Extending the trend of twelve closely agreeing values by the least squares procedure to zero sodium ion concentration while ignoring five high scattered values gives a  $\log K$  of 5.87 which is in good agreement with the value of 66P at zero ionic strength.

The nmr measurements of 84P were made at a rather large ligand concentration (5mM) which makes the results questionable because of the expected ligand stacking and intermolecular metal complex bonding.

The calorimetric results of 69B, and presumably also those of 82S from the same research group, used a rather large ligand concentration (2.5mM) and values calculated from the difference with two different metal ion concentrations would also be questionable because of intermolecular bonding. The intermolecular bonding would be expected to be considerably changed when the metal ion concentration is doubled for the second part of the measurement.

There is some question as to the precision of the values of 66P. In Table II of that paper the value of 4.63 is listed as the average of three separate determinations at 25°C and 0.10 M ionic strength but the value listed in Table VI is 4.60. Moreover use of their zero ionic strength value adjusted to 0.10 M with their equation gives 4.55, and the values in Table II for 0.065 and 0.17 M ionic strength adjusted to 0.10 M agree at 4.53. It would seem that the average of the experimental values adjusted to 0.10 M at  $4.56 \pm 0.04$  would best represent their results and this value is included as the selected constant in Table 3.

The ion exchange values of 57N were determined at a ligand concentration too high for this method (see 58W) and the same worker obtained a higher value after remeasurement at a lower concentration (61N).

The potentiometric values of 62T and of 66Pa showed that use of a ten-fold excess of metal ion concentration would lower the formation constants with ATP. Consequently values based on excess metal ion (56M, 56Sa, 58Wa, and 62H) were not further considered. No information about metal ion concentration was given in 76R and 78R but since their values agreed with those having excess metal ion, it was presumed that excess metal ion was used there also.

The spectrophotometric work of 64O involving the use of three different buffers gave three different values after conversion to 0.10 M ionic strength, which suggests that the amine type buffers complex magnesium ion more strongly than has been thought or that the protonated buffer complexes with the deprotonated ligand (see 77N). Therefore the reported constants involving the use of a large concentration of NEM or TRIS in measuring this complex (61N(ix), 63W, 64O, 70N, 73L, 74E, 77N, 81B, 84J, 85J) were not further considered.

Insufficient experimental details are given in 58M, in 68N, in 80K, or in 80V to evaluate the reported values and they were not further considered.

The results of 73Sa are based upon the addition of magnesium ion to ATP and assuming that the protons released are equivalent to the amount of magnesium ion bound but at the pH values employed, only a fraction of the ligand is protonated and the assumption is not correct.

The potentiometric results of 61N are similar to the above in that magnesium ion is added to ATP and the pH change is used to calculate the constant. The assumption is made that the measured pH is equal to the protonation constant but this becomes less accurate as the pH differs from the mid-point of the buffer region and all of the experimental results in the paper obtained by this method show an increase in the constant to a maximum and then a decrease. The low and high values were then averaged but the maximum near 4.56 is probably the more precise result where the assumption made is justified. This result agrees with the selected values given below.

The spectrophotometric values of 78A are dependent upon the pH employed, with decreasing values as the pH is lowered. Use of the protonation equilibrium of ATP does not correct for the pH dependence, which indicates that additional factors change as the pH changes. The results of 71B, 79M, 81B, and 81W are probably low because of the low pH used. The authors of 78A feel that their spectrophotometric results are in error because of the large pH variance and prefer their ion selective electrode (ise) values. Their ise value for

pH 7.0 agrees with their value at pH 8.0 after converting to 0.10 M ionic strength and correcting for pH but their value at pH 9.0 does not agree.

The remaining values are 64O(gl) at 4.82, 78Gb(4.67), 86C(4.72), and 87S(4.64) averaging to  $4.68 \pm 0.04$ , 59B(4.58), 61N(max)(4.56), 62T(4.51), 63W(TEA)(4.54), 64O(TEA)(4.60), 66P(4.56), 73Ba(4.50), 78A(ise)(4.56), 78M(4.59), and 88G(4.60) agreeing at  $4.55 \pm 0.05$ , 72F(4.46) and 87Sa(4.38) agreeing at  $4.42 \pm 0.04$ , and 79M at 4.26. The greater agreement is at 4.55 and this is recommended for the  $Mg^{2+}$  complex with ATP. The value of 86D(4.60) calculated from the literature is in approximate agreement after converting from  $Pr_4N^+$  to  $Me_4N^+$  medium.

The average of the 66P value and the recalculated 74M value at 5.85 is recommended for MgATP at zero ionic strength.

The value at 1.00 M ionic strength by 76R appears to be low relative to the 0.10 M values. The value of 88G for 0.50 M ionic strength is tentatively recommended.

#### Calcium Complexes of ATP

Values for the  $Ca^{2+}$  complex with ATP have been reported in twenty three papers with a range from 5.28 to 3.21 after conversion of the published values to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complexes.

The values of 72M were corrected for sodium ion by the use of a large constant for the NaATP complex and are probably over-corrected. Consecutive values in Table I of that paper seem to show a dependence upon sodium ion concentration, especially points 11,12,13,14,15 and 17,18,19. There is too much scatter in the plot against sodium ion concentration to get a meaningful extrapolation to zero. The value of the NaATP complex used for correction in 85O is that of 72M and led to over-correction since the calcium complexation constant is higher than all other calcium values.

The values of 56Sa, 56M, and 78R are probably low because of excess metal ion concentration; those of 57N because the ligand concentration was too large for the method used as with MgATP; that of 85J because of competition from sulfate ions; that of 64O(sp) because of buffer complexation; those of 61N(sp,ix) and of 79B because of the low pH used; and that of 61N(gl) because of the assumption that the hydrogen ion concentration is the same as the protonation constant. There are too few details in 80K to evaluate the constant and therefore it is considered doubtful.

Elimination of the above values leaves 59B(4.47) and 64O(4.47) in agreement, 86C(4.38) somewhat lower, 62T(4.26), 78M(4.23), 87S(4.26), and 88G(4.20) in agreement, 87Sa at 4.05, and 58W(3.79) and 86D(3.76) agreeing much lower but the agreement between the groups is not very good. The average of the ten of sixteen differences between the MgATP and CaATP values for those who measured both under the same conditions is  $0.33 \pm 0.08$ . This comparison predicts  $4.55 - 0.33 = 4.22 \pm 0.08$ , which is in agreement with the average of 62T, 78M, 87S, and 88G at  $4.24 \pm 0.02$  and therefore 4.24 is recommended for the value of the  $Ca^{2+}$  complex with ATP.

The higher ionic strength values of 84G and 86D are apparently low relative to the 0.10 M values but the 0.50 M ionic strength value of 88G is tentatively recommended.

#### Strontium and Barium Complexes of ATP

For the  $Sr^{2+}$  and  $Ba^{2+}$  complexes of ATP, after exclusion of 56Sa because of the large metal ion concentration used, 61N because of the assumption that hydrogen ion concentration is the same as the protonation constant, 60O because of lack of experimental details, and 86C because of high constants for MgATP and for CaATP, the values of 62T, adjusted by the same amount as the difference between its CaATP value and the recommended value, are tentatively recommended.

#### Protonated Complexes of MATP

The MHL complex of  $Mg^{2+}$  with HATP has been reported in fourteen papers. The work of 62T shows that excess metal ion would produce low results and those who used excess magnesium ion (56M, 56Sa, 58Wa, and 62H) are probably low because of this. The ML values of 64O, 79Mc, and 84P are higher than the recommended value and MHL values would be expected to be high also. This leaves 66P at 2.7, 87S at 2.42, 62T(2.24), 72F(2.23), and 88G(2.2) agreeing at 2.22, 87Sa at 2.12, and 86C at 1.94. The average of 87S, 62T, 72F, and 88G at  $2.32 \pm 0.10$  is recommended for the complex of  $Mg^{2+}$  with HATP.

The complex of  $Ca^{2+}$  with HATP has been reported in nine papers. The value of 56Sa is low with MgHATP and is probably low here. The use of a buffer and the low pH in 62A would give a low value. This leaves 86C at 2.31, 62T(2.13), 79Mc(2.12), and 87S(2.20) agreeing at  $2.16 \pm 0.04$ , 87Sa at 2.04, 88G at 1.99, and 86D at 1.61. The average of three of six differences between MgHATP and CaHATP is  $0.17 \pm 0.06$  which predicts  $2.32 - 0.17 = 2.15 \pm 0.10$ . This agrees with the majority average and 2.16 is recommended for  $Ca^{2+} + HATP$ .

Since the values of 56Sa are low with MgHATP and with CaHATP, 86C is low for MgHATP and high with CaHATP, and the values of 62T agree with the recommended values, the values of 62T, adjusted by the same amount as the difference between its MgHATP value and the recommended value, are tentatively recommended for the  $Sr^{2+}$ , and  $Ba^{2+}$  complexes with HATP.

The values of 88G at 0.50 M ionic strength are tentatively recommended for MgHATP and for CaHATP.

### Binuclear Complexes of ATP

The binuclear complex,  $Mg_2ATP$ , is needed to explain the kinetic results of 72Fa and others. After excluding the value of 74M because of the use of a high NaATP constant to correct for sodium ion, and 88G with a very low value, the average of the other five values of 59B, 70Na, 72Fa, 81B, and 82S at  $1.7 \pm 0.1$  is recommended for adding a second  $Mg^{2+}$  to MgATP.

Two of the three papers that report values for the binuclear complex,  $Ca_2ATP$ , have high values for CaATP and would be expected to be high here while 88G is low for  $Mg_2ATP$  and appears to be low here too. Therefore these values are not recommended.

### Magnesium Complexes of AQP

The values for the  $Mg^{2+}$  complexes with AQP by 57S were apparently determined in an excess of magnesium ion and since an excess with ATP gives a low value (62T) and there is a greater charge on AQP, these values are probably low and are not recommended. Also the MgAQP-MgHAQP difference (1.5) does not fit the trend of MgADP-MgHADP difference (1.6) to MgATP-MgHATP (2.0).

### Alkaline Earth Metal Complexes of Other Nucleotide Triphosphates

For magnesium and calcium complexes with nucleotide triphosphates other than ATP, the values of 73S were not used because of the assumption that protons released were equivalent to magnesium ions bound; the values of 58W because of being low with ATP; and those of 73T and 83R because of the large variations with different nucleotide triphosphates while similar values would be expected because of the common triphosphate group.

The average value of 72F(4.44), 77S(4.43), and 87S adjusted to the recommended ATP value (4.46) at 4.44 is recommended for the  $Mg^{2+}$  complex with CTP. The values of 77S, adjusted to the MgCTP value, are tentatively recommended for the  $Mg^{2+}$  complex with GTP(4.49) and with ITP(4.44). The average values of 77S adjusted and 87S adjusted are tentatively recommended for MgUTP(4.43) and for MgTTP(4.50).

For  $Ca^{2+} + CTP$ , the average of 77S(4.07) and 87S, adjusted to the ATP value, (4.18) at 4.13 is tentatively recommended. The average values of 77S and 87S, both adjusted to the CaCTP value are tentatively recommended for CaUTP(4.14) and for CaTTP(4.16). The 77S values, adjusted to CaCTP, are tentatively recommended for CaGTP(4.14) and for CaITP(4.14).

The MHL value of 72E(2.22) supported by that of 87S adjusted to the recommended HATP value (2.2  $\pm$  0.2) is recommended for  $Mg^{2+} + HCTP$ . The values of 73S for MgHGTP(2.31) and for MgHITP(2.34) are tentatively recommended. The average of 73S(2.54) and adjusted 87S (2.61) at 2.58 is recommended for MgHUTP.

The 87S values adjusted to the recommended HATP value are tentatively recommended for CaHCTP(2.17) and for CaHUTP(2.70).

The MHL value of 72F for  $Mg^{2+}$  with CTP is tentatively recommended. The 83R values for  $Mg^{2+}$  and  $Ca^{2+}$  with CTP seem much too large compared to those of other nucleotide triphosphates and are not recommended. The MHL values of 73S for  $Mg^{2+}$  with GTP, ITP, and UTP are not recommended because of the assumption that the protons released are equivalent to the magnesium ions bound.

The binuclear complex of 72Fa for  $Mg^{2+}$  with MgCTP rounded off to 1.8 is tentatively recommended.

### Alkaline Earth Metal Complexes of ADP

The formation constant for the  $Mg^{2+}$  complex with ADP has been reported in twenty four papers and after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complexes, the range of values is from 4.2 to 2.74.

The values of 69B, 70B, 78A(sp), 78Ga, and 84P are high for MgATP and are probably high with ADP for the same reasons. The value of 74F is probably high because of the use of a large constant for the NaADP complex to correct for the presence of sodium ion. The values of 57N, 64O, 74E, and 77N are low for MgATP and are probably low with ADP for the same reasons. The values of 56M and 56Sa are low for MgATP and MgAMP-5 and are probably low with ADP also. The value of 82V is probably low because of the low pH and the use of a TRIS buffer. The values of 84G are higher for some complexes than those of most other workers and lower for other complexes, which suggests that this work contains experimental or computational errors. The conditions used in 83C are uncertain and the value appears to be low. No temperature is given in 80K and in 83G and their values were not considered. The values of 58W and 58Wa are low with MgATP but agree with the recommended values with ADP.

The average of the five remaining values, 59B(3.36), 62T(3.31), 66P(3.50), 72F(3.43), and 87Sa(3.54), at 3.43 is recommended for the  $Mg^{2+}$  complex with ADP. The average of the remaining thirteen differences of the values of MgATP and MgADP after disregarding the five lowest differences for those who measured both equilibria is  $1.1 \pm 0.1$  which predicts  $4.55 - 1.1 = 3.45 \pm 0.1$  and supports the recommended value.

Thirteen papers have reported values for the  $Ca^{2+}$  complex with ADP which range from 3.93 to 2.54 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complexes.

The value of 74F is probably over-corrected because of the use of a large constant for NaADP; that of 57N is low because of the use of a too high ligand concentration for the method used; that of 84G is based on a very large protonation constant and its MgADP value is too low; that of 83G may be low because of the low pH, the TRIS buffer, and a possible tertiary complex involving the metal ion indicator; that of 79B may be low because of the low pH, the buffer used, and the competing chelator; that of 62A is probably low because of the low pH, the buffer used, and the low CaATP value; that of 56Sa is probably low since the MgADP value is very

low; that of 59B is probably low since it agrees with two others that are expected to be low (56Sa, 62A); and that of 56M is probably low since the corresponding values for ATP and AMP-5 are low.

The average of the remaining values, 58W(3.09), 62T(3.00), 64O(3.08), and 87Sa(3.16) at  $3.08 \pm 0.08$  is recommended for the  $\text{Ca}^{2+}$  complex with ADP. The nine differences between the MgATP and MgADP values, for those who measured both, have an average of  $0.3 \pm 0.1$  which predicts  $3.40 - 0.3 = 3.10 \pm 0.1$  and supports the recommended value.

The values of 62T, adjusted the same as the difference between their CaADP value and the recommended CaADP value, are tentatively recommended for the  $\text{Sr}^{2+}$  and  $\text{Ba}^{2+}$  complexes with ADP.

The values of 72F for the  $\text{Mg}^{2+}$  complex with CDP and of 58W, adjusted the same as the difference between their MgADP value and the recommended MgADP value, for the  $\text{Mg}^{2+}$  complex with UDP are tentatively recommended. The 73S values for the  $\text{Mg}^{2+}$  complex with GDP and with UDP are too large relative to the recommended ADP value and if adjusted to the MgADP value from the same research group (69B) are too small and not recommended.

For the MHL complex of  $\text{Mg}^{2+}$  with HADP, after omission of 84P because of high values for MgADP and MgHATP; of 66P because of a high value with MgHATP; of 56M and 56Sa because of low values with MgADP and MgHATP; the remaining values are 87Sa at 1.90 and 58Wa(1.58), 62T(1.64), and 72F(1.60) agreeing at  $1.61 \pm 0.03$ . The latter average is recommended for MgHADP. The value of 72F(1.62) for MgHCDP is tentatively recommended.

The values of 62T, after adjustment to the average of the MgHADP values, are tentatively recommended for the  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  complexes with HADP. The value of 87Sa for CaHADP (0.59) seems much too low.

After omitting the value of 74F because of the use of a large NaADP constant, the value of 72Fa, 1.0, is tentatively recommended for the binuclear complex of  $\text{Mg}^{2+}$  with MgADP. The value of the binuclear complex of 72Fa for  $\text{Mg}_2\text{CDP}$ , 1.0, is also tentatively recommended. The value of 74F for  $\text{Ca}_2\text{ADP}$  is not recommended because of the large NaADP constant used.

#### Alkaline Earth Metal Complexes of AMP

Values for the alkaline earth metal complexes of AMP-5 have been reported in fourteen papers. Those of 56M and 56Sa are low with ATP and with ADP and are probably low here. The values of 64S and 88Sa are about the same magnitude as these two and therefore probably too small. The large NaAMP-5 value used by 76K to correct for sodium ions and the obtaining of a larger value for CaAMP-5 than for MgAMP-5, contrary to all other comparisons, make the reported values suspect. The too large ligand concentration of 57N for the method used makes the reported constant suspect. The assumption that the protons released are equivalent to the magnesium ion bound makes the value of 69B questionable. The value of 77N is also probably in error because of the low pH and TRIS buffer used. The value of 60O for SrAMP-5 appears to be low and has too few details for evaluation.

For the  $\text{Mg}^{2+}$  complex with AMP-5, the above considerations leave 58Wa and 87Sa agreeing at 2.23, and 58W(2.09), 62Ta(2.06), 72F(1.94), and 79T(2.01) agreeing at 2.02 after conversion from a potassium or sodium ion background. The average of the six remaining differences between the MgADP and MgAMP-5 values, after omission of a very large difference (69B) and of the smallest difference (57N), is  $1.4 \pm 0.1$  which predicts  $3.43 - 1.4 = 2.03 \pm 0.1$ , which is in agreement with the majority and 2.02 is therefore recommended.

The average of 58W(1.90) and 62Ta(1.94) at 1.92, after correction for  $\text{Na}^+$  or  $\text{K}^+$  complexes, is recommended for  $\text{Ca}^{2+}$  + AMP-5. The value of 87Sa is higher (2.26) and their value is also high with MgAMP-5. For the  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  complexes with AMP-5, the values of 62T adjusted relative to the magnesium value are tentatively recommended. The trend from MgAMP-5 to CaAMP-5 and from SrAMP-5 to BaAMP-5 is about the same for 62Ta and for 89M but while that of 62Ta from CaAMP-5 to SrAMP-5 conforms to that expected from ionic size, that of 89M is inconsistent.

Since 62Ta values were used for the AMP-5 values and the 58Wa and 89M (same workers as 88Sa) values were not, the 62Ta values adjusted to the MgAMP-5 average are tentatively recommended for the  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  complexes with AMP-3.

For AMP-2, the average of 67T(2.02) and 72F(1.89) at 1.96 is recommended for the  $\text{Mg}^{2+}$  complex and the adjusted values of 67T are tentatively recommended for the  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  complexes for internal consistency. The trend from AMP-3 to AMP-2 to AMP-5 is linear with similar differences for both 62Ta-67T and for 89M.

Adjustment of the other monophosphate values to the recommended value of MgAMP-5, based on values in the same paper (72F,79T) or by the same method from the same research group (73S on 69B, 84S,88M,88Ma on 88Sa), gives values in close agreement. Therefore the average of 73S(1.97) and 79T(2.00) at 1.99 for MgGMP-5; of 72F(1.96), 79T(1.89), and 88M(1.92) at 1.93 for MgCMP-5; of 73S(1.91), 84S(1.90), and 88M(1.98) at 1.94 for MgUMP-5; and of 79T(1.95) and 88M(1.97) at 1.96 for MgTMP-5 are recommended.

The values of 88M, adjusted in the same manner as was employed for the magnesium complexes, are tentatively recommended for  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , and  $\text{Ba}^{2+}$  complexes with CMP-5, UMP-5, and TMP-5. The value of 88Ma for CaGMP-5(1.99) seems a little too large relative to MgGMP-5 and to CaAMP-5 and is not recommended.

The MHL values of 79T for  $\text{Mg}^{2+}$  with AMP-5, with GMP-5, with TMP-5, and with CMP-5 are not recommended because of the inaccuracy of measuring such small constants by the potentiometric method.

## Transition Metal Complexes

### Manganese Complexes

Values for the stability constant of the Mn(II) complex of ATP have been reported in twenty three papers with a range from 5.90 to 4.17 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The values of 77R are considerably larger than all of the other values, probably because of the assumption that the quantity of protons released when metal ions are added is equivalent to the metal ions bound to the ligand, which would not be true at the pH employed. The same method also gave high values for the MgATP constant (73S).

The values of 74M, 78Ga, 79Mc, and 86C are high for MgATP and are probably high for Mn(II) for the same reasons. There are too few experimental details in 80K to evaluate the constant and it was not further considered. The values of 56Sa, 62H, 78R, and 85J are low for MgATP and are probably low here for the same reasons. The value of 73V is probably low because of competition for the manganese ion by the relatively high concentration of the sodium cacodylate buffer used. The value of 84G is questionable because of the large protonation constant used in the calculations. The ion exchange and electron paramagnetic resonance results of 70J are probably low because of the use of a NEM buffer. The results of 64O with MgATP were low with this buffer and a greater effect would be expected here because of the stronger bonding of the manganese ion.

The remaining values are 78M(5.26) and 87S(5.36) agreeing at  $5.31 \pm 0.05$ , and 58W(5.12), 61B(5.09), 62T(5.07), 66Pa(5.15), 77Sa(5.05), 80Db(5.14), and 83J(5.16) agreeing at  $5.11 \pm 0.06$ . The average of seven of twelve differences between MgATP and MnATP values of those who measured both is  $0.57 \pm 0.1$  which predicts  $4.55 + 0.57 = 5.12 \pm 0.1$  in agreement with the majority and therefore 5.11 is recommended for the  $Mn^{2+}$  complex with ATP in 0.10 M  $Me_4N^+$  media.

The ten MHL values range from 3.70 to 1.67 after adjusting to 25°C and 0.10 M ionic strength. The value of 74M is probably overcorrected for sodium ions; that of 79Mc is probably high because of the large protonation constant used; that of 86C is probably high since their values are also high for CaATP and ZnATP; that of 56Sa is probably low for the same reason that the MgATP and MnATP values are low; and that of 80Db is probably high because of the high value reported for ZnATP. This leaves 83J at 2.85, 87S at 2.74, 62H(2.64) and 66Pa(2.59) agreeing at 2.62, and 62T at 2.39. The average of 62H, 66Pa, and 87S at  $2.65 \pm 0.09$  is recommended for the complex of  $Mn^{2+}$  with HATP. Four of six differences between MgHATP and MnHATP average to  $0.2 \pm 0.1$  which predicts  $2.31 + 0.2 = 2.7 \pm 0.1$ , five of ten differences between MnATP, with no sodium or potassium complexes, and MnHATP averages to  $2.5 \pm 0.1$  which predicts  $5.11 - 2.5 = 2.6 \pm 0.1$ , and support the selected value.

With other nucleotide triphosphates, the values of 73T and 83R fluctuate from high values with some complexes compared to other workers to low values with other complexes which suggests that there are experimental or computational errors in these reports. The value of 84M with MnCTP is probably low because of the use of a too small protonation constant.

The average of the values of 58W(5.10) and 77S(4.99) for the  $Mn^{2+}$  complexes with GTP at  $5.05 \pm 0.06$ , that of 77Sa, adjusted by the same amount that is necessary to change their MnATP value to the recommended value for MnATP, with ITP (5.07), the average of 58W(5.14), 77S(5.09), and 87S, adjusted by the difference between their MnATP value and the recommended value of ATP, (5.00) with CTP at  $5.07 \pm 0.07$ , the average of 58W(5.15) and adjusted 87S (5.01) with UTP at  $5.08 \pm 0.07$ , and that of adjusted 87S at 5.1 for TTP are recommended. The values of 58W for MnITP(4.94) and 77S for MnUTP(4.93) seem low relative to the other Mn values in the same papers and to the recommended Mn values. The values of 87S, adjusted by the difference between their MnHATP value and the recommended MnHATP value, for MnHCTP( $3.0 \pm 0.3$ ) and for MnHUTP(2.62) are tentatively recommended.

Values for the complex of  $Mn^{2+}$  with ADP have been reported in nine papers and range from 4.41 to 3.42 after conversion to 25°C, 0.10 M ionic strength and correction for sodium or potassium complex formation.

The value of 77R is high with MnATP and is probably high here for the same reason. Likewise 56Sa is low with MnATP and probably low here. The values of 80Db and 84G are based upon high protonation constants and are questionable. The value of 84G is low with MgADP and probably low here. The ion exchange constant of 70J agrees with the high value of 77R and is therefore questionable.

The remaining values of 58W(4.22), 62Ta(4.36), 64O(sp)(4.22), 64O(epr)(4.26), 70J(epr)(4.31), and 78Gb(4.22) agree at  $4.29 \pm 0.07$ . The average of four out of six differences between the MgADP and the MnADP values is  $0.84 \pm 0.10$  which predicts  $3.43 + 0.84 = 4.27 \pm 0.10$  and the average of nine out of eleven differences between the MnATP and MnADP values is  $0.8 \pm 0.2$  which predicts  $5.11 - 0.8 = 4.3 \pm 0.2$ . These differences support 4.29, which is recommended for the complex of  $Mn^{2+}$  with ADP in 0.10 M  $Me_4N^+$  media.

The values of 56Sa are too low for MgHADP and for SrHADP and the MnHADP value appears to be low. The 80Db value appears to be high relative to most other MHL values with ADP. Therefore the MHL value of 62Ta is tentatively recommended for  $Mn^{2+} + HADP$ .

The value of 84M for the  $Mn^{2+}$  complex with CDP is probably low because of the use of a protonation constant that is 0.2 units low and is not recommended.

Values for the  $Mn^{2+}$  complex with AMP-5 have been reported in nine papers with a range from 2.49 to 2.11 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The values of 56Sa, 64S, and 88Sa are low for the MgAMP-5 complex and are probably low here for the same reasons. The value of 80Db is low for MnADP and is lower than all other values here. The value of 77R is questionable because of the assumption that the protons released are equivalent to the manganese bound. The value of 61T is probably low because of the large quantity of buffer used, which could complex with the manganese ions.

The average of the remaining values of 58W(2.45), 62Ta(2.49), and 66D(2.44) is  $2.46 \pm 0.03$ . The average of four differences between MgAMP-5 and MnAMP-5 is  $0.45 \pm 0.06$  which predicts  $2.02 + 0.45 = 2.47 \pm 0.06$  and the average of three out of four differences between MnADP and MnAMP-5 is  $1.84 \pm 0.05$  which predicts  $4.29 - 1.84 = 2.45 \pm 0.05$ . These support the value of 2.46 which is recommended for the  $Mn^{2+}$  complex with AMP-5 in 0.10 M  $Me_4N^+$  media.

For the complexes of  $Mn^{2+}$  with AMP-3 and with AMP-2, the average of values of 62Ta and 67T, adjusted by the difference between their MnAMP-5 value and the recommended MnAMP-5 value, (2.34, 2.44) and 89M adjusted the same way (2.29, 2.37) are recommended. The value of 66D for MnAMP-3 seems much too low.

The 88M values for MnCMP-5, MnUMP-5, and MnTMP-5, adjusted the same as the difference between the 89M values and the recommended values with MnAMP-3 and with MnAMP-2, are tentatively recommended. The values of 84M and 85K for MnCMP-5 seem high and that of 84S for MnUMP-5 seems low compared to the recommended MnAMP-5 value.

### Iron (II) Complexes

The values of 78R are low with MgATP, MnATP, CoATP, NiATP, CuATP, and ZnATP but the FeATP value is much higher than would be expected compared to the other transition metal complexes and may involve partial oxidation to iron (III). The 71R value at 1.00 M ionic strength seems to be high relative to those at 0.10 M for the other transition metal complexes. Therefore no iron (II) values are recommended.

### Cobalt Complexes

Values for the complex of  $Co^{2+}$  with ATP have been reported in fourteen papers with a range from 7.07 to 4.4 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The ion exchange results of 75K are considerably larger than all of the other values and may be in error because of the very large ligand concentration relative to the metal ion concentration. The results of 78Ga are probably high because of the assumption that the protons released are equivalent to the amount of cobalt ion bound. The results obtained with this method were also high with MnATP(77R) and with MgATP(73S). The values of 86C are high for the other transition metal complexes with ATP and is probably high here also. The values of 78R and 85J are low with MnATP and are probably low here for the same reasons. The values of 60B and 61B may be low because of complexation by sulfate ions. The value of 80Da is based on an incorrect protonation constant and appears to be too low.

The remaining values are 87S at 5.32, 66Pa(5.17) and 67S(5.21) agreeing at 5.19 and 58W(4.97), 62T(4.95), and 64H(4.95) agreeing at 4.96. The average difference between MnATP and CoATP of six out of nine differences is  $0.06 \pm 0.09$  which predicts  $5.11 - 0.06 = 5.05 \pm 0.09$ . The average of five differences between MgATP and CoATP is  $0.56 \pm 0.1$  which predicts  $4.55 + 0.56 = 5.11 \pm 0.1$ . These differences are between the two groups and suggest that there is a rather large uncertainty with this complex and an overall average of  $5.1 \pm 0.1$  is recommended for the  $Co^{2+}$  complex with ATP in 0.10 M  $Me_4N^+$  media.

For the MHL complex, the values are 87S at 2.8, 80Da at 2.73, 66Pa at 2.63, 86C at 2.60, and 62T at 2.32. The average of three of five differences between MnHATP and CoHATP is  $0.0 \pm 0.1$  which predicts  $2.65 + 0.0 = 2.65 \pm 0.1$ . This agrees with the average of 80Da, 66Pa, and 86C at  $2.66 \pm 0.07$  and therefore 2.66 is recommended for  $Co^{2+} + HATP$ .

With the other nucleotide triphosphates, the value of 58W, adjusted by the difference between their CoATP value and the recommended CoATP value, at 5.11 for CoGTP; the average of 58W(5.11) and 77C(5.16) at 5.13 for CoITP; the average value of adjusted 58W(4.96), 84M(4.98), and adjusted 87S(4.91) at 4.95 for CoCTP; the average value of adjusted 58W(5.03), 78F(4.88), adjusted 87S(4.86) at 4.95 for CoUTP; and adjusted 87S at 4.91 for CoTTP are recommended. The average value of 87S, adjusted by the difference between their CoHATP value and the recommended CoHATP value, (2.9) and 84M(2.58) at 2.8 is recommended for  $Co^{2+}$  with HCTP, while that of adjusted 87S at 2.5 is tentatively recommended for  $Co^{2+}$  with HUTP.

The complex of  $Co^{2+}$  with ADP has been measured in five papers and the values range from 6.12 to 3.71 after adjustment to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The value of 75K was high for CoATP and is very high here. The value of 80Db was low for MnADP and appears to be too low here as well. The values of 58W and of 80M agree at 3.94 but this would give a large drop from the recommended MnADP value which is contrary to the ATP and AMP-5 differences and is very unlikely. Therefore the remaining value of 62Ta at 4.40 is tentatively recommended for the complex of  $Co^{2+}$

with ADP in 0.10 M  $\text{Me}_4\text{N}^+$  media. The difference of 84M between MnCDP and CoCDP agrees with the difference of 62Ta between MnADP and CoADP.

For the MHL complex of  $\text{Co}^{2+}$  with HADP, the value of 62Ta at 2.01 is tentatively recommended because of the uncertainty of the 80Db and 80M values.

The value of 84M at 4.07 for the  $\text{Co}^{2+}$  complex with CDP appears to be low and the MHL value at 2.4 appears to be high and are not recommended.

The values of the  $\text{Co}^{2+}$  complex with AMP-5 have been reported in nine papers and range from 3.44 to 2.32 after adjustment to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The value of 75K is high with CoATP and with CoADP and appears to also be high here. The results of 64S, 80Da (same workers as 80Db), and 88Sa are low for MnAMP-5 and are probably low here as well. The value of 80M is low for CoADP and is low here too. The remaining values of 58W(2.71), 62Ta(2.62), 66D(2.66), and 77P(2.53) agree at  $2.62 \pm 0.09$ . The five differences between MnAMP-5 and CoAMP-5 average  $0.19 \pm 0.08$  which predicts  $2.46 + 0.19 = 2.65 \pm 0.08$ , in agreement with the average. Therefore 2.62 is recommended for the complex of  $\text{Co}^{2+}$  with AMP-5 in 0.10 M  $\text{Me}_4\text{N}^+$  media.

The MHL value reported by 77P for CoHAMP-5 seems high and is not recommended.

The average of 62Ta(2.29), 66D(2.15)(adjusted the same as the difference between their CoAMP-5 value and the recommended value), and 89M(2.19)(adjusted the same way) at 2.22 is recommended for CoAMP-3 in 0.10 M  $\text{Me}_4\text{N}^+$  media. Similarly, the average of 67T(2.33) and adjusted 89M(2.32) at 2.32 is recommended for CoAMP-2. The values of 88M for CoCMP-5, CoUMP-5, and CoTMP-5, adjusted the same as the difference between the 89M values and the recommended values with CoAMP-3 and with CoAMP-2, are tentatively recommended. The values of 84M and 85K appear to be high for CoCMP-5. The MHL value of 66D for CoHAMP-3 is too small for accurate measurement by potentiometry and is not recommended.

### Nickel Complexes

Values for the complex of  $\text{Ni}^{2+}$  with ATP have been reported in ten papers with a range from 5.31 to 4.85 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The values of 60B, 78R, and 80D are low for the CoATP complex and are probably low here also. The value of 61B is lower than these and must be too low. The median of the other values, 62T(5.31), 64H(5.3), 66Pa(5.31), 67S(5.20), 72F(5.12), and 87S(5.21), at  $5.21 \pm 0.10$  is recommended for the complex of  $\text{Ni}^{2+}$  with ATP in 0.10 M tetramethylammonium medium. The average of three of four differences between MgATP and NiATP for those who measured both is  $0.68 \pm 0.1$  which predicts  $4.55 + 0.68 = 5.23 \pm 0.1$  and supports the value of 5.21.

The MHL values are 66Pa at 2.97, 87S at 2.86, 72F at 2.80, 62T at 2.72, and 80D at 2.61. The three differences between MgHATP and NiHATP average to  $0.50 \pm 0.07$  which predicts  $2.31 + 0.50 = 2.81 \pm 0.10$  which supports the average of 87S, 72F, and 62T at  $2.79 \pm 0.07$  and that is recommended for  $\text{Ni}^{2+} + \text{HATP}$ .

The values of 77C at 5.08 for NiITP; the average value of 72F, adjusted by the difference between their NiATP value and the recommended ATP value, (4.88), 84M(4.80), and 87S(4.82) at 4.84 for NiCTP; and the values of 87S for NiUTP at 4.82 and for NiTTP at 4.87 are recommended. The values of 73T and of 83R are not recommended. The average of the MHL values of 72F, 84M, and 87S at 2.7 is recommended for the complex of  $\text{Ni}^{2+}$  with HCTP and that of adjusted 87S at 2.4 is tentatively recommended for NiHUTP.

Four papers have reported values for  $\text{Ni}^{2+}$  with ADP. The values of 79M and 80D are low with NiAMP-5 and appear to be low here also. The average of 62Ta (adjusted by the difference between their MnADP value and the recommended MnADP value to become 4.63), and 72F(4.42) at  $4.5 \pm 0.1$  is recommended for the complex of  $\text{Ni}^{2+}$  with ADP in 0.10 M tetramethylammonium medium.

After eliminating the 80D value which appears to be much too low, the average of 62Ta(2.30), 72F(2.32), and 79M(2.32) at 2.31 is recommended for the complex of  $\text{Ni}^{2+}$  with HADP.

The values of 72F, adjusted to the recommended NiADP value, at 3.82 for NiCDP and at 1.89 for NiHCDP are tentatively recommended.

Eleven papers have reported values for  $\text{Ni}^{2+}$  with AMP-5 with values from 2.93 to 2.43 after correction to 25°C, 0.10 M ionic strength, and adjustment for sodium or potassium complex formation. The same workers as those in 79M, with the same method are low with MnAMP-5(77R), CoAMP-5(80M), and NiADP and those of 80D are low with MnAMP-5(80Db), CoAMP-5(80Da), CuAMP-5, NiADP, and NiATP and are probably low with NiAMP-5 for the same reasons. The values of 62Ta are 0.09 higher than the recommended value for NiATP and 0.13 higher than NiADP, which suggests that NiAMP-5 should be about  $2.93 - 0.11 = 2.82$ . The values of 72F are 0.10 lower than NiATP and 0.08 lower than NiADP which suggests that NiAMP-5 should be about  $2.62 + 0.09 = 2.71$ . The median of 2.82 and 2.71 is about the same as the 64S(2.75) and the 66D(2.76) values and suggest 2.76 for NiAMP-5. The average of the differences between the 88Sa values and the recommended values for MnAMP-5, CoAMP-5, CuAMP-5, and ZnAMP-5 is  $0.14 \pm 0.1$  which suggests  $2.62 + 0.14 = 2.76 \pm 0.1$  for NiAMP-5. The three differences between CuAMP-5 and NiAMP-5, where both were reported in the same paper, average to  $0.44 \pm 0.10$  which predicts  $3.22 - 0.44 = 2.78 \pm 0.10$  and the three differences between NiATP and NiAMP-5, with no sodium or potassium complexes, average to  $2.44 \pm 0.06$  which predicts  $5.21 - 2.44 = 2.78 \pm 0.10$ . These differences support 2.76 and this is recommended for NiAMP-5 in 0.10 M tetramethylammonium medium.

For NiAMP-3 and NiAMP-2, the values of 62Ta are close to those for NiAMP-5 while the values of 72F, 76Ta, 80Ta, and 89M show a decrease of about 0.6 to NiAMP-3 and about 0.5 to NiAMP-2. The trend of these differences for  $Mn^{2+}$  and for  $Co^{2+}$  in 62Ta shows an increasing difference from AMP-5 to AMP-3 of 0.12 and 0.33, which supports the 0.6 difference for  $Ni^{2+}$ . Therefore the values of 80Ta, adjusted by the difference between their NiAMP-5 value and the recommended value of NiAMP-5, are recommended for NiAMP-3(2.24) and NiAMP-2(2.34). The value of adjusted 76Ta is in excellent agreement with the former and that of adjusted 72F is in approximate agreement with the latter. The values of 89M are slightly lower but their  $Co^{2+}$ - $Ni^{2+}$  differences are similar to those between the recommended values.

The values of 85K are high for MnCMP-5, CoCMP-5, and CuCMP-5 and the NiCMP-5 value is higher than the other three values. The value of 81N for NiIMP-5 seems high relative to the other  $Ni^{2+}$  complexes. The MHL values reported for AMP-5, for AMP-3, for AMP-2, and for CMP-5 are too low for accurate determination by the potentiometric method and are not recommended.

The values of 88M, adjusted according to the difference between their 89M value with NiAMP-2 and the recommended value, are tentatively recommended for NiCMP-5(2.34), for NiUMP-5(2.37) and for NiTMP-5(2.32). The 80O value for NiCMP-5, from the same research group, is in good agreement while the 72F value is lower.

### Copper Complexes

Stability constants for the  $Cu^{2+}$  complex of ATP have been reported in seventeen papers which range from 6.86 to 5.80 after conversion to 25°C, 0.10 M ionic strength, and correcting for sodium or potassium complex formation.

The values for 60B, 61B, 78R, and 80D are low for CoATP and NiATP and are probably low for Cu(II) also. Those for 62H are low for MgATP and MnATP and appear to be low here also. The value of 83A agrees with the low values and also appears to be low with ZnATP while the constant corrected for potassium complexes in the paper is probably over-corrected because of the use of a constant good for small amounts of potassium ion but not for the large excess employed during the measurements (see Alkali Metal Complexes discussion). The use of large protonation constants in 79Mc and in 84G probably mean that these constants are too large. The values of 86C were too large with the other transition metals and appear to be too large here as well.

The remaining constants are in two groups, 64Sa(6.66), 66Pa(6.82), 67S(6.73), 85T(6.67), and 87S(6.69) agreeing at  $6.74 \pm 0.08$ , and 62T(6.42), 78M(6.38), and 83W(6.46) agreeing at  $6.42 \pm 0.04$ . Seven out of nine differences between MgATP and CuATP, for those who measured both, average to  $1.9 \pm 0.1$  which predicts  $4.55 + 1.9 = 6.45 \pm 0.1$  and seven of eleven differences between MnATP and CuATP average to  $1.3 \pm 0.1$  which predicts  $5.11 + 1.3 = 6.41 \pm 0.1$ . The two sets of differences agree with the group reporting the lower constants and therefore 6.42 is recommended for the complex of  $Cu^{2+}$  with ATP in 0.10 M tetramethylammonium medium.

The MHL values from eleven papers range from 3.79 to 2.91 after conversion to 25°C and 0.10 M ionic strength. The values for 66Pa, 85T, 86C, and 87S are high for CuATP and would be expected to be high here while that of 83A is low and would be expected to be low here. This leaves 79Mc(3.59) and 80D(3.62) agreeing at  $3.60 \pm 0.02$ , 83W(3.45) and 86C(3.43) agreeing at  $3.44 \pm 0.01$ , 62H at 3.25, and 62T at 3.12. Four of five differences between MgHATP and CuHATP have a median of  $1.03 \pm 0.1$  which predicts  $2.31 + 1.03 = 3.34 \pm 0.1$ . Four of seven differences between MnHATP and CuHATP have a median of  $0.73 \pm 0.1$  which predicts  $2.65 + 0.73 = 3.38 \pm 0.1$ . The median of 62H, 83W, and 86C( $K^+$ ) at  $3.35 \pm 0.10$  agrees with these differences and is recommended for  $Cu^{2+} + HATP$ .

For the other nucleotide triphosphates, the values of 77S at 6.28 for CuGTP; of 77C at 6.34 for CuITP; of the average of 77S(6.1), 84M(5.93), and 87S, adjusted by the difference between their CuATP value and the recommended CuATP value, (6.11) at 6.02 for CuCTP; of the average of adjusted 87S(3.56) and 84M(3.42) at 3.49 for CuHCTP; of 78F(5.88), 85T(6.16), and adjusted 87S(5.95) at 6.0 for CuUTP; of 85T at 2.8 for CuHUTP; and of the average of 77S(6.05), and adjusted 87S(5.9) at 6.0 for CuTTP are tentatively recommended.

The 84G values for MgADP, CaADP, and MnADP are low and CuADP appears to be low also. With 80D, the NiADP, NiATP, NiAMP-5, and CuAMP-5 values are low and the CuADP value is probably low. Therefore the only other value (62Ta), adjusted by the difference between their MnADP value and the recommended MnADP value, is tentatively recommended. The CuCDP value of 84M seems low and the CuHCDP value of 84M seems high relative to the recommended CuADP values and are not recommended.

Only two MHL values have been reported for ADP but the 80D value is not dependable since the values from this group range from very high to very low and therefore the value of 62Ta at 2.63 is tentatively recommended for the complex of  $Cu^{2+}$  with HADP.

Five values have been reported for the complex of  $Cu^{2+}$  with AMP-5 but the values from the researchers of 80D (80Da, 80Db) are low with MnAMP-5, CoAMP-5, and NiAMP-5 and appear to be low here. This leaves 88A at 3.7 and 62Ta(3.27), 64S(3.17), and 88Sa(3.27) agreeing at  $3.22 \pm 0.05$ . The later value of 3.22 is recommended for CuAMP-5.

The average of 62Ta(3.05) and 89M(2.88) is recommended for CuAMP-3 and that of 67T(3.25) and 89M(3.14) at  $3.20 \pm 0.06$  for CuAMP-2. The values of 88M for CuCMP-5, the average of 84S and 88M for



CuUMP-5, and of 88M for CuTMP-5 are tentatively recommended. The values of 58Wa and 84M for CuCMP-5 seem high relative to the CuAMP-5 value and are therefore not recommended.

The higher ionic strength value of 84G(0.50 M) seems high and that of 76R(1.00 M) seems low relative to the 0.10 M ionic strength values and are not recommended.

### Zinc Complexes

Seventeen papers have reported values for the  $Zn^{2+}$  complex with ATP which range from 7.56 to 4.4 after conversion to 25°C, 0.10 M ionic strength, and correction for sodium or potassium complex formation.

The value of 78K is much larger than all of the other values and must be too large. The values of 84G and of 86C are too large for MgATP and CuATP and also appear to be too large here. The values of 78R and of 85J are too small with MgATP, MnATP, and CoATP and are much too small here. The value of 83A is low for CuATP and appears to be low here while the corrected value is probably over-corrected as with CuATP. Because of a large protonation constant, the 79Mc values are high with MgATP, MnATP, and CuATP, and would be expected to be high here. The values of 58Wa and of 62H are based upon the use of a large excess of zinc ions and would be expected to be low. This leaves 66Pa(5.47), 67S(5.56), 78M(5.45), and 87S(5.51) agreeing at  $5.50 \pm 0.06$  and 61B(5.12), 62T(5.14), 80Db(5.21), and 85M(5.21) agreeing at  $5.16 \pm 0.05$ . Eight of fourteen differences between CuATP and ZnATP, for those who measured both, average to  $1.25 \pm 0.10$  which predicts  $6.42 - 1.25 = 5.17 \pm 0.10$  and supports the smaller constant at 5.16 which is recommended for ZnATP.

At higher ionic strengths, the value of 84G at 0.50 M seems high and that of 76R at 1.00 M seems very low compared to the values at 0.10 M ionic strength and are not recommended.

The eleven MHL values range from 3.62 to 2.08 after conversion to 25°C and 0.10 M ionic strength. After eliminating 66Pa, 86C, and 87S for being high with ML and 62H and 83A for being low with ML, the others are 80Db at 2.94, and 58Wa(2.75), 62T(2.67), and 79Mc(2.64) agreeing at  $2.69 \pm 0.06$ . Three differences between NiHATP and ZnHATP average to  $0.04 \pm 0.04$  which predicts  $2.79 - 0.04 = 2.75 \pm 0.07$  and six of nine differences between CuHATP and ZnHATP average to  $0.7 \pm 0.2$  which predicts  $3.35 - 0.7 = 2.65 \pm 0.2$ . These values support the average of 58Wa, 62T, and 79Mc at 2.69, which is recommended for  $Zn^{2+} + HATP$ .

For the other nucleotide triphosphates, the average values of 77S(5.14), 84M(5.08), and 87S, adjusted by the difference between their ZnATP value and the recommended ATP value, (5.03) at 5.09 for ZnCTP; of 84M(2.9) and adjusted 87S(2.88) at 2.88 for ZnHCTP; of 78F(5.10) adjusted 87S(5.01) at 5.06 for ZnUTP and at 2.56 for ZnHUTP; of 77S(5.24) and adjusted 87S(5.03) at 5.1 for ZnTTP; are recommended.

Four papers report values for ZnADP but the value of 84G is very low for MnADP and for CuADP and appears to be high here and the value of 80Db is low for MnADP and for CoADP and appears to be low here also. Therefore the average of 58Wa(4.33) and 62Ta(4.48) at  $4.41 \pm 0.08$  is recommended for the complex of  $Zn^{2+}$  with ADP.

Three values for ZnHADP have been reported but the 80Db value is undependable since the MnHADP value is very high and the CoHADP value is very low. The two remaining values have poor agreement but since 62Ta values are recommended for MnHADP, CoHADP, NiHADP, and CuHADP the value of 62Ta at 2.04 for the  $Zn^{2+}$  complex with HADP is tentatively recommended for consistency.

The 84M value for ZnCDP is based on a small protonation constant, appears to be low, and is not recommended. The MHL value of 84M appears to be high relative to that of ZnADP and is not recommended.

Five values with no agreement have been reported for ZnAMP-5. The value of 78K is very high for ZnATP and is very high here relative to the other AMP-5 constants with metal ions. The 64S value is very low for CoAMP-5 and this value seems much too low relative to the recommended CoAMP-5 and NiAMP-5 values. The 88Sa values are low for MnAMP-5, NiAMP-5, and CoAMP-5 and are low here relative to the recommended values of MnAMP-5, CoAMP-5, and NiAMP-5. Therefore the 62Ta value, adjusted to the average difference between the 62T values and the recommended values for MnAMP-5, CoAMP-5, NiAMP-5, and CuAMP-5, to become 2.77, is tentatively recommended for the complex of  $Zn^{2+}$  with AMP-5.

The complex of ZnAMP-3 has been reported in four papers but the agreement is not good. The average of the two middle values of 66D(2.57) and 62Ta(2.65)(adjusted by the difference between their ZnAMP-5 value and the recommended ZnAMP-5 value) at  $2.61 \pm 0.04$  is recommended for the complex of  $Zn^{2+}$  with AMP-3. The value of 67T, adjusted to become 2.69, is tentatively recommended for the complex of  $Zn^{2+}$  with AMP-2.

The values of 88M for ZnCMP-5, 84S and 88M for ZnUMP-5, and 88M for ZnTMP-5, adjusted the same as the difference between the 89M value for ZnAMP-2 and the recommended value for ZnAMP-2, are tentatively recommended. The value of 85K for ZnCMP-5 is in good agreement. The values of 58Wa and 84M seem too high for ZnCMP-5.

### Cadmium Complexes

The values of 60B are low for CoATP, NiATP, and CuATP and would be expected to be low for CdATP. The 84P value is even lower, the 84C value involved a wrong protonation constant, and 85B used a large excess of  $Cd^{2+}$ . Therefore the average of 84Sa and 87S (from the same research group) at 5.68 is tentatively recommended for  $Cd^{2+} + ATP$  at 25°C, 0.10 M ionic strength, and corrected for sodium or potassium complex formation.

The average of 84Sa and 87S at 3.00 is tentatively recommended for  $\text{Cd}^{2+} + \text{HATP}$  as well as for  $\text{Cd}^{2+} + \text{CTP}$  at 5.33 and  $\text{Cd}^{2+} + \text{HCTP}$  at 3.16. The values of 87S at 5.41 for  $\text{CdUTP}$ , at 2.89 for  $\text{CdHUTP}$ , and at 5.34 for  $\text{CdTTP}$  are tentatively recommended.

The 84P values for  $\text{CdATP}$  are low and the  $\text{CdADP}$  values appear to be low and are not recommended.

The values of 88M, 88Sa, and 89M, after adjusting the same as the  $\text{Zn}^{2+}$  values differ from the recommended  $\text{Zn}^{2+}$  values, are tentatively recommended for  $\text{CdCMP-5}$ , for  $\text{CdUMP-5}$ , and for  $\text{CdTMP-5}$ . The value of 88Ma for  $\text{CdGMP-5}$  is much larger than the above values and is not recommended.

#### Other Metal Complexes

The  $\text{Be}^{2+}$  value with  $\text{ATP}$  is not recommended because other values from the same paper are low.

With  $\text{Sc}^{3+}$ ,  $\text{Y}^{3+}$ , and lanthanide ions, some formation constants were measured in buffers which would give low values (73V, 74E, 80Ma, 83M), assume that hydrogen ions released are equivalent to the  $\text{Eu}^{3+}$  bound (78G), or give too few details for evaluation (70B). The trends with atomic number of the 87Sb values are more similar to those observed with other ligands than are the 88R values. Therefore the 87Sb values, after correction for sodium complex formation, are tentatively recommended.

The  $\text{Fe}^{3+}$  values of 68R are based on high protonation constants and are not recommended.

The  $\text{VO}^{2+}$  values with  $\text{ATP}$  and with  $\text{ADP}$  varied with pH, which shows that they are not properly defined and are not recommended.

The  $\text{Ti}^{+}$  values with  $\text{ATP}$  and with  $\text{ADP}$  are tentatively recommended after adjustment to 0.10 M  $\text{Na}^{+}$  (+0.11), as discussed under the alkali metal constants, and then to 0.10 M  $\text{Me}_4\text{N}^{+}$  (+0.35 for  $\text{ATP}$ , +0.26 for  $\text{ADP}$ ), as discussed under the protonation constants and with the assumption that the effect is the same because of identical charges.

The  $(\text{CH}_3)_3\text{Sn}^{+}$  values for  $\text{AMP-5}$  and for  $\text{IMP-5}$  are described by different sets of equilibria and the one common equilibrium (ML) lists the  $\text{IMP-5}$  value as much smaller than the  $\text{AMP-5}$  value which would not be expected and therefore these values are not recommended.

With  $\text{Al}^{3+}$ , there are not enough details in 80V for proper evaluation, the results of 87J indicate a much larger value for  $\text{Al}^{3+} + \text{ADP}$  than for  $\text{Al}^{3+} + \text{ATP}$ , and consequently no values are recommended.

### V. RECOMMENDED VALUES

The recommended metal formation constants are collected in Table 6 with an estimate of the uncertainty for each value.

The nucleotide formation constants, especially with transition metals, presented difficulties in the selection process which suggests that other variables are affecting the results. One possibility is that the metal ions catalyze the hydrolysis of the ligands. Therefore the use of fresh ligand solutions and expeditious measurements after the addition of metal ions may be important. Ligand and metal ion concentrations may be significant in the variability of results. Higher concentrations give ligand stacking and intermolecular metal complex bonding while excessive metal ions may give polynuclear complexes. Therefore concentrations below one millimolar may be necessary for unambiguous determination of mononuclear complex stability constants. Impurities in the nucleotides, such as hydrolysis products, which vary with preparation and time since preparation, may contribute to the variability. Analysis and purification of the ligand before use should reduce this uncertainty.

Evaluation of minor species, which are especially important with  $\text{CuATP}$  and with  $\text{ZnATP}$ , was not attempted because of the difficulties in selecting major species and the expected variation of their magnitudes with the particular set of equilibria chosen.

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**Table 4. Recommended Nucleotide Protonation and Complexation Enthalpy Changes (25°C, 0.10 M, kJ/mol)**

Ligand	Equilibrium	$\Delta H$				
		$H^+ + L$	$Mg^{2+} + L$	$Ca^{2+} + L$	$Eu^{3+} + L$	
ATP	ML/M.L	-0.8 ± 0.8(R)	+18.8 ± 0.8(R)	+14.2 ± 0.8(T)	+42 ± 4(T)	
	MHL/M.HL	-15.0 ± 0.8(R)	+9.6 ± 0.8(R)	+7.9 ± 0.8(T)		
GTP	ML/M.L	-0.4 ± 2 (T)	+18.0 ± 0.8(T)			
	MHL/M.HL	-13 ± 4 (T)				
ITP	ML/M.L	-1.3 ± 2 (T)	+18.8 ± 0.8(T)			
	MHL/H.HL	-8 ± 4 (T)				
CTP	ML/M.L	-0.4 ± 2 (T)				
	MHL/M.HL	-21 ± 4 (T)				
UTP	ML/M.L	+0.4 ± 2 (T)	+18.4 ± 0.8(T)			
	MHL/M.HL	-21 ± 4 (T)				
ADP	ML/M.L	-2.9 ± 2 (R)	+13.4 ± 0.8(T)		+21 ± 4(T)	
	MHL/M.HL	-17.2 ± 1 (R)	+7.5 ± 1 (T)	+6.3 ± 1 (T)		
GDP	ML/M.L	-1.7 ± 2 (T)	+14.2 ± 0.8(T)			
	MHL/M.HL	-13 ± 4 (T)				
IDP	ML/M.L	-2.5 ± 2 (T)				
	MHL/M.HL	-8 ± 4 (T)				
CDP	ML/M.L	-2.5 ± 2 (T)				
	MHL/M.HL	-21 ± 4 (T)				
UDP	ML/M.L	-3.3 ± 2 (T)	+13.4 ± 0.8(T)			
	MHL/M.HL	-21 ± 4 (T)				
AMP-5	ML/M.L	-4.2 ± 2 (R)	+7.5 ± 0.8(T)	+4.2 ± 1 (T)	0 ± 4(T)	
	MHL/M.HL	-17.6 ± 1 (R)				
AMP-3	ML/M.L	-2.9 ± 2 (T)	+7.9 ± 2 (T)			
	MHL/M.HL	-16.3 ± 2 (T)				
AMP-2	ML/M.L	-3.3 ± 2 (T)	+7.9 ± 2 (T)			
	MHL/M.HL	-16.7 ± 2 (T)				
GMP-5	ML/M.L	-1.7 ± 2 (T)	+7.1 ± 0.8(T)			
	MHL/M.HL	-13 ± 4 (T)				
IMP-5	ML/M.L	-2.1 ± 2 (T)				
	MHL/M.HL	-8 ± 4 (T)				
CMP-5	ML/M.L	-2.1 ± 2 (T)				
	MHL/M.HL	-21 ± 4 (T)				
UMP-5	ML/M.L	-3.3 ± 2 (T)	+7.5 ± 0.8(T)			
	MHL/M.HL	-21 ± 4 (T)				

  

Ligand	Equilibrium	$\Delta H$				
		$Li^+ + L$	$Na^+ + L$	$K^+ + L$	$Rb^+ + L$	$Cs^+ + L$
ATP	ML/M.L	-4 ± 4 (T)	-0.8 ± 0.8(T)	+1.3 ± 0.8(T)	+4 ± 4 (T)	+8 ± 4 (T)

  

Ligand	Equilibrium	$\Delta H$				
		$Mn^{2+} + L$	$Co^{2+} + L$	$Ni^{2+} + L$	$Cu^{2+} + L$	$Zn^{2+} + L$
ATP	ML/M.L	+18.0 ± 0.2(T)	+18.8 ± 0.8(T)	[+12] ± 3 (T)	+3.3 ± 0.8(T)	+16.3 ± 0.8(T)
	MHL/M.HL			-14.6 ± 0.8(T)	+4.6 ± 0.8(T)	
	M2L/ML.M			+18.0 ± 0.8(T)	+12.6 ± 0.8(T)	
ADP	ML/M.L	+13.4 ± 0.8(T)	+11.7 ± 2 (T)	+6.3 ± 0.8(T)	[-1.3] ± 3 (T)	[+10.5] ± 3 (T)
AMP-5	ML/M.L	+9.2 ± 0.8(T)	-0.4 ± 2 (T)	-10.5 ± 0.8(T)	[-17] ± 4 (T)	[-4] ± 4 (T)
AMP-3	ML/M.L	+9.6 ± 2 (T)	-2.5 ± 3 (T)	-10.0 ± 2 (T)	[-17] ± 4 (T)	[-4] ± 4 (T)
AMP-2	ML/M.L	+9.2 ± 2 (T)	-2.1 ± 3 (T)	-10.0 ± 2 (T)	[-17] ± 4 (T)	[-4] ± 4 (T)

[ ] = estimated value based on trends. (R) = recommended value. (T) = tentatively recommended value.  
± = estimated uncertainty of recommended value.

Table 5. Recommended Nucleotide Protonation Constants\* (log K, 25°C)

Ligand	Equilibrium	Log K in 0.10 M Pr <sub>4</sub> N <sup>+</sup>	Log K in 0.10 M Et <sub>4</sub> N <sup>+</sup>	Log K in 0.10 M Me <sub>4</sub> N <sup>+</sup>	Log K in 0.10 M K <sup>+</sup>	Log K in 0.10 M Na <sup>+</sup>
AQP	HL/H.L	7.46 ± 0.05(T)	7.42 ± 0.05(T)	7.25 ± 0.05(T)	6.77 ± 0.05(R)	6.65 ± 0.05(T)
	H <sub>2</sub> L/H.HL				4.05 ± 0.05(T)	
ATP	HL/H.L	6.96 ± 0.05(R)	6.93 ± 0.07(R)	6.79 ± 0.07(R)	6.50 ± 0.06(R)	6.44 ± 0.08(R)
	H <sub>2</sub> L/H.HL	4.03 ± 0.05(T)	3.99 ± 0.06(T)	3.96 ± 0.08(T)	4.02 ± 0.08(R)	3.98 ± 0.10(R)
	H <sub>3</sub> L/H.H <sub>2</sub> L					1.8 ± 0.1 (R)
GTP	L/H.(H <sub>-1</sub> L)					9.68 ± 0.05(T)
	HL/H.L	6.95 ± 0.05(T)				6.37 ± 0.08(R)
	H <sub>2</sub> L/H.HL				3.0 ± 0.1 (T)	
ITP	L/H.(H <sub>-1</sub> L)					9.15 ± 0.05(T)
	HL/H.L	7.01 ± 0.05(T)				6.37 ± 0.05(R)
	H <sub>2</sub> L/H.HL				2.2 ± 0.1 (T)	
CTP	HL/H.L	6.99 ± 0.05(T)			6.55 ± 0.09(R)	6.45 ± 0.05(R)
	H <sub>2</sub> L/H.HL					4.43 ± 0.05(T)
UTP	L/H.(H <sub>-1</sub> L)					9.59 ± 0.05(T)
	HL/H.L	6.90 ± 0.05(T)				6.42 ± 0.08(R)
	H <sub>2</sub> L/H.HL					1.9 ± 0.1 (T)
TTP	L/H.(H <sub>-1</sub> L)					9.78 ± 0.05(T)
	HL/H.L					6.40 ± 0.05(T)
ADP	HL/H.L	6.65 ± 0.05(R)	6.63 ± 0.05(R)	6.55 ± 0.05(R)	6.36 ± 0.05(R)	6.31 ± 0.09(R)
	H <sub>2</sub> L/H.HL				3.95 ± 0.05(T)	3.94 ± 0.05(R)
GDP	HL/H.L	6.71 ± 0.05(T)				6.2 ± 0.1 (T)
	H <sub>2</sub> L/H.HL					2.8 ± 0.1 (T)
IDP	HL/H.L	6.69 ± 0.05(T)				
CDP	HL/H.L	6.68 ± 0.05(T)			6.40 ± 0.05(T)	6.3 ± 0.1 (T)
	H <sub>2</sub> L/H.HL				4.45 ± 0.05(T)	
UDP	HL/H.L	6.68 ± 0.05(T)				6.4 ± 0.1 (T)
AMP-5	ML/H.L	6.35 ± 0.05(R)	6.34 ± 0.05(T)	6.29 ± 0.02(R)	6.21 ± 0.02(R)	6.18 ± 0.08(R)
	H <sub>2</sub> L/H.HL			3.79 ± 0.07(T)	3.80 ± 0.07(R)	3.80 ± 0.07(R)
AMP-3	ML/H.L				5.80 ± 0.05(R)	5.72 ± 0.06(R)
	H <sub>2</sub> L/H.HL				3.64 ± 0.05(R)	3.60 ± 0.06(R)
AMP-2	ML/H.L				6.01 ± 0.05(R)	5.85 ± 0.06(T)
	H <sub>2</sub> L/H.HL				3.70 ± 0.06(R)	3.64 ± 0.06(T)
GMP-5	ML/H.L	6.39 ± 0.05(T)				6.20 ± 0.06(R)
	H <sub>2</sub> L/H.HL					2.32 ± 0.06(R)
GMP-3	M2L/H.HL					2.15 ± 0.06(T)
IMP-5	ML/H.L	6.34 ± 0.05(T)			6.19 ± 0.05(T)	
CMP-5	ML/H.L	6.31 ± 0.05(T)			6.27 ± 0.04(R)	6.15 ± 0.06(R)
	H <sub>2</sub> L/H.HL				4.32 ± 0.08(R)	4.31 ± 0.09(R)
CMP-3	M2L/H.HL					4.24 ± 0.09(T)
UMP-5	L/H.(H <sub>-1</sub> L)					9.39 ± 0.08(R)
	HL/H.L	6.34 ± 0.04(T)				6.04 ± 0.09(T)
TMP-5	L/H.(H <sub>-1</sub> L)					9.79 ± 0.08(T)
	HL/H.L					6.24 ± 0.09(T)

\* These are concentration constants using hydrogen ion concentration. Mixed constants may be obtained from these values by using an activity coefficient of 0.78 which increases them by 0.11 units.

Table 5 (continued)

Ligand	Equilibrium	Log <i>K</i> at	Log <i>K</i> at
		25°, -0	37°, 0.15 M Na <sup>+</sup>
ATP	HL/H.L	7.68 ± 0.05(T)	6.40 ± 0.08(R)
	H <sub>2</sub> L/H.HL		3.92 ± 0.05(R)
	H <sub>3</sub> L/H.H <sub>2</sub> L	1.91 ± 0.05(T)	
GTP	HL/H.L	7.65 ± 0.05(T)	
ITP	HL/H.L	7.68 ± 0.05(T)	
CTP	HL/H.L	7.65 ± 0.05(T)	
UTP	HL/H.L	7.58 ± 0.05(T)	
ADP	HL/H.L	7.20 ± 0.05(T)	6.27 ± 0.05(R)
	H <sub>2</sub> L/H.HL		3.82 ± 0.05(R)
GDP	HL/H.L	7.19 ± 0.05(T)	
IDP	HL/H.L	7.18 ± 0.05(T)	
CDP	HL/H.L	7.18 ± 0.05(T)	
UDP	HL/H.L	7.16 ± 0.05(T)	
AMP-5	ML/H.L	6.67 ± 0.05(T)	6.14 ± 0.05(R)
	H <sub>2</sub> L/H.HL		3.67 ± 0.06(R)
GMP-5	ML/H.L	6.66 ± 0.05(T)	
IMP-5	ML/H.L	6.66 ± 0.05(T)	
CMP-5	ML/H.L	6.62 ± 0.05(T)	
UMP-5	ML/H.L	6.63 ± 0.05(T)	

  

Ligand	Equilibrium	Log <i>K</i> at	Log <i>K</i> at	Log <i>K</i> at
		25°, 0.25M (Medium)	25°, 0.50M (Medium)	25°, 1.00M (Medium)
ATP	HL/H.L	6.93 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )	6.98 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )	7.14 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )
		6.88 ± 0.05(R) (Et <sub>4</sub> N <sup>+</sup> )	6.91 ± 0.05(T) (Et <sub>4</sub> N <sup>+</sup> )	7.03 ± 0.05(T) (Et <sub>4</sub> N <sup>+</sup> )
		6.73 ± 0.05(T) (Me <sub>4</sub> N <sup>+</sup> )	6.69 ± 0.05(T) (Me <sub>4</sub> N <sup>+</sup> )	6.72 ± 0.05(T) (Me <sub>4</sub> N <sup>+</sup> )
		6.34 ± 0.05(T) (K <sup>+</sup> )	6.16 ± 0.05(T) (K <sup>+</sup> )	6.03 ± 0.06(R) (K <sup>+</sup> )
		6.27 ± 0.05(T) (Na <sup>+</sup> )	6.07 ± 0.05(T) (Na <sup>+</sup> )	5.93 ± 0.05(T) (Na <sup>+</sup> )
		3.98 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )	4.04 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )	4.19 ± 0.05(T) (Pr <sub>4</sub> N <sup>+</sup> )
	H <sub>2</sub> L/H.HL	3.95 ± 0.05(T) (Et <sub>4</sub> N <sup>+</sup> )		
		3.96 ± 0.05(T) (Me <sub>4</sub> N <sup>+</sup> )		
		3.98 ± 0.05(T) (K <sup>+</sup> )	3.98 ± 0.05(T) (K <sup>+</sup> )	3.99 ± 0.05(R) (K <sup>+</sup> )
		3.98 ± 0.05(T) (Na <sup>+</sup> )	3.99 ± 0.05(R) (Na <sup>+</sup> )	4.00 ± 0.05(R) (Na <sup>+</sup> )

(R) = recommended value. (T) = tentatively recommended value. ± = estimated uncertainty of recommended value.

**Table 6. Recommended Nucleotide Metal Ion Complexation Constants (log K, 25°C, 0.10 M Me<sub>4</sub>N<sup>+</sup>)**

Ligand	Equilibrium	Li <sup>+</sup>	Na <sup>+</sup>	K <sup>+</sup>	Rb <sup>+</sup>	Cs <sup>+</sup>
AQP	ML/M.L	2.22 ± 0.05(T)	1.71 ± 0.05(T)	1.54 ± 0.05(T)		
ATP	ML/M.L	1.78 ± 0.08(R)	1.31 ± 0.03(R)	1.17 ± 0.03(R)	1.11 ± 0.05(T)	1.06 ± 0.05(T)
ADP	ML/M.L	1.32 ± 0.05(T)	1.12 ± 0.04(R)	1.00 ± 0.05(R)		
AMP-5	ML/M.L	1.22 ± 0.05(T)	0.88 ± 0.07(R)	0.70 ± 0.06(R)		
Ligand	Equilibrium	Mg <sup>2+</sup>	Ca <sup>2+</sup>	Sr <sup>2+</sup>	Ba <sup>2+</sup>	
ATP	ML/M.L	4.55 ± 0.07(R)	4.24 ± 0.07(R)	3.82 ± 0.07(T)	3.57 ± 0.07(T)	
	MHL/M.HL	2.32 ± 0.10(R)	2.16 ± 0.07(R)	2.08 ± 0.10(T)	1.88 ± 0.10(T)	
	M2L/M.ML	1.7 ± 0.1 (R)				
GTP	ML/M.L	4.49 ± 0.07(T)	4.14 ± 0.07(T)			
	MHL/M.HL	2.31 ± 0.05(T)				
ITP	ML/M.L	4.44 ± 0.07(T)	4.14 ± 0.07(T)			
	MHL/M.HL	2.34 ± 0.10(T)				
CTP	ML/M.L	4.44 ± 0.07(R)	4.13 ± 0.07(T)			
	MHL/M.HL	2.22 ± 0.10(T)	2.17 ± 0.10(T)			
	M2L/M.ML	1.8 ± 0.1 (T)				
UTP	ML/M.L	4.43 ± 0.07(T)	4.14 ± 0.07(T)			
	MHL/M.HL	2.58 ± 0.10(R)	2.70 ± 0.10(T)			
TTP	ML/M.L	4.50 ± 0.07(T)	4.16 ± 0.07(T)			
ADP	ML/M.L	3.43 ± 0.10(R)	3.08 ± 0.08(R)	2.76 ± 0.08(T)	2.58 ± 0.08(T)	
	MHL/M.HL	1.61 ± 0.03(R)	1.65 ± 0.10(T)	1.60 ± 0.10(T)	1.51 ± 0.10(T)	
	M2L/M.ML	1.0 ± 0.1 (T)				
CDP	ML/M.L	3.44 ± 0.10(T)				
	MHL/M.HL	1.62 ± 0.10(T)				
	M2L/M.ML	1.0 ± 0.1 (T)				
UDP	ML/M.L	3.35 ± 0.10(T)				
AMP-5	ML/M.L	2.02 ± 0.10(R)	1.92 ± 0.10(R)	1.84 ± 0.10(T)	1.78 ± 0.10(T)	
AMP-3	ML/M.L	1.94 ± 0.10(T)	1.85 ± 0.10(T)	1.76 ± 0.10(T)	1.74 ± 0.10(T)	
AMP-2	ML/M.L	1.98 ± 0.10(R)	1.88 ± 0.10(T)	1.79 ± 0.10(T)	1.76 ± 0.10(T)	
GMP-5	ML/M.L	1.99 ± 0.10(R)				
CMP-5	ML/M.L	1.93 ± 0.10(R)	1.86 ± 0.10(T)	1.77 ± 0.10(T)	1.72 ± 0.10(T)	
UMP-5	ML/M.L	1.94 ± 0.10(R)	1.90 ± 0.10(T)	1.85 ± 0.10(T)	1.74 ± 0.10(T)	
TMP-5	ML/M.L	1.96 ± 0.10(R)	1.86 ± 0.10(T)	1.79 ± 0.10(T)	1.72 ± 0.10(T)	
Ligand	Equilibrium	Mn <sup>2+</sup>	Co <sup>2+</sup>	Ni <sup>2+</sup>	Cu <sup>2+</sup>	Zn <sup>2+</sup>
ATP	ML/M.L	5.11 ± 0.07(R)	5.1 ± 0.1 (R)	5.21 ± 0.10(R)	6.42 ± 0.07(R)	5.16 ± 0.07(R)
	MHL/M.HL	2.65 ± 0.09(R)	2.66 ± 0.07(R)	2.79 ± 0.07(R)	3.35 ± 0.10(R)	2.69 ± 0.06(R)
GTP	ML/M.L	5.05 ± 0.07(R)	5.11 ± 0.07(T)		6.28 ± 0.07(T)	
ITP	ML/M.L	5.07 ± 0.07(T)	5.13 ± 0.07(R)	5.08 ± 0.07(T)	6.34 ± 0.07(T)	
CTP	ML/M.L	5.08 ± 0.08(R)	4.95 ± 0.07(R)	4.84 ± 0.07(R)	6.02 ± 0.07(R)	5.09 ± 0.07(R)
	MHL/M.HL	3.0 ± 0.3 (T)	2.8 ± 0.2 (T)	2.7 ± 0.1 (R)	3.49 ± 0.07(R)	2.88 ± 0.07(R)
UTP	ML/M.L	5.08 ± 0.07(R)	4.95 ± 0.09(R)	4.82 ± 0.07(T)	6.0 ± 0.1 (R)	5.06 ± 0.07(R)
	MHL/M.HL	2.62 ± 0.09(T)	2.5 ± 0.2 (T)	2.4 ± 0.1 (T)	2.8 ± 0.1 (T)	2.56 ± 0.07(T)
TTP	ML/M.L	5.1 ± 0.1 (T)	4.91 ± 0.07(T)	4.87 ± 0.07(T)	6.0 ± 0.1 (R)	5.1 ± 0.1 (R)
ADP	ML/M.L	4.29 ± 0.07(R)	4.40 ± 0.07(T)	4.5 ± 0.1 (R)	6.03 ± 0.07(T)	4.41 ± 0.07(R)
	MHL/M.HL	1.89 ± 0.10(T)	2.01 ± 0.10(T)	2.31 ± 0.05(R)	2.63 ± 0.10(T)	2.04 ± 0.10(T)
AMP-5	ML/M.L	2.46 ± 0.07(R)	2.62 ± 0.07(R)	2.76 ± 0.07(R)	3.22 ± 0.07(R)	2.76 ± 0.07(T)
AMP-3	ML/M.L	2.32 ± 0.07(R)	2.22 ± 0.07(R)	2.24 ± 0.07(R)	2.97 ± 0.09(R)	2.61 ± 0.07(R)
AMP-2	ML/M.L	2.41 ± 0.07(R)	2.32 ± 0.07(R)	2.34 ± 0.07(T)	3.20 ± 0.07(R)	2.69 ± 0.07(T)
CMP-5	ML/M.L	2.36 ± 0.07(T)	2.28 ± 0.07(T)	2.34 ± 0.07(R)	2.97 ± 0.07(T)	2.42 ± 0.07(T)
UMP-5	ML/M.L	2.37 ± 0.07(T)	2.29 ± 0.07(T)	2.37 ± 0.07(R)	2.90 ± 0.07(T)	2.38 ± 0.07(T)
TMP-5	ML/M.L	2.37 ± 0.07(T)	2.31 ± 0.07(T)	2.32 ± 0.07(R)	3.00 ± 0.07(T)	2.46 ± 0.07(T)

Table 6 (continued)

Ligand	Equilibrium	Cd <sup>2+</sup>		Tl <sup>+</sup>	Y <sup>3+</sup>	
ATP	ML/M.L	5.68 ± 0.07(T)		2.5 ± 0.1 (T)		6.64 ± 0.07(T)
	MHL/M.HL	3.00 ± 0.07(T)				3.64 ± 0.07(T)
CTP	ML/M.L	5.29 ± 0.07(T)				
	MHL/M.HL	3.16 ± 0.07(T)				
ADP	ML/M.L			1.7 ± 0.1 (T)		
AMP-5	ML/M.L	3.04 ± 0.07(T)				4.48 ± 0.07(T)
	MHL/M.HL					2.76 ± 0.07(T)
CMP-5	ML/M.L	2.53 ± 0.07(T)				
UMP-5	ML/M.L	2.51 ± 0.07(T)				
TMP-5	ML/M.L	2.55 ± 0.07(T)				

  

Ligand	Equilibrium	La <sup>3+</sup>	Nd <sup>3+</sup>	Eu <sup>3+</sup>	Dy <sup>3+</sup>	Tm <sup>3+</sup>
ATP	ML/M.L	6.32 ± 0.07(T)	6.58 ± 0.07(T)	6.66 ± 0.07(T)	6.72 ± 0.07(T)	6.80 ± 0.07(T)
	MHL/M.HL	3.52 ± 0.07(T)	3.63 ± 0.07(T)	3.65 ± 0.07(T)	3.66 ± 0.07(T)	3.67 ± 0.07(T)
AMP-5	ML/M.L	3.91 ± 0.07(T)	4.22 ± 0.07(T)	4.63 ± 0.07(T)	4.70 ± 0.07(T)	4.59 ± 0.07(T)
	MHL/M.HL	2.76 ± 0.07(T)	2.74 ± 0.07(T)	2.72 ± 0.07(T)	2.71 ± 0.07(T)	2.70 ± 0.07(T)

(log K, 37°C, 0.15 M Na<sup>+</sup>)

  

Ligand	Equilibrium	Na <sup>+</sup>	Mg <sup>2+</sup>	Ca <sup>2+</sup>
ATP	ML/M.L	0.83 ± 0.10(R)	4.34 ± 0.07(R)	3.99 ± 0.07(R)
	MHL/M.HL		2.39 ± 0.07(R)	2.21 ± 0.07(T)
ADP	ML/M.L	0.71 ± 0.10(R)	3.22 ± 0.07(R)	2.85 ± 0.07(R)
	MHL/M.HL		1.57 ± 0.07(R)	1.52 ± 0.07(T)
AMP-5	ML/M.L	0.36 ± 0.10(R)	1.92 ± 0.10(R)	1.68 ± 0.10(T)

  

Ligand	Equilibrium	Mn <sup>2+</sup>	Co <sup>2+</sup>	Ni <sup>2+</sup>	Cu <sup>2+</sup>	Zn <sup>2+</sup>
ATP	ML/M.L	4.79 ± 0.07(R)	4.8 ± 0.1 (R)	4.86 ± 0.07(R)	5.99 ± 0.07(R)	4.83 ± 0.07(R)
	MHL/M.HL				2.90 ± 0.07(R)	2.61 ± 0.07(R)
ADP	ML/M.L	4.08 ± 0.07(R)	4.18 ± 0.07(T)	4.2 ± 0.1 (R)	5.71 ± 0.07(T)	4.18 ± 0.07(R)
AMP-5	ML/M.L	2.38 ± 0.07(R)	2.48 ± 0.07(R)	2.6 ± 0.1 (R)	2.94 ± 0.07(R)	2.58 ± 0.07(T)

(log K, 25°C, corrected for background electrolyte)

  

Ligand	Equilibrium	Mg <sup>2+</sup> , -0	Mg <sup>2+</sup> , 0.50 M	Ca <sup>2+</sup> , 0.50 M
ATP	ML/M.L	5.85 ± 0.07(R)	4.50 ± 0.07(T)	4.10 ± 0.07(T)
	MHL/M.HL		2.1 ± 0.1 (T)	1.93 ± 0.10(T)

(R) = recommended value. (T) = tentatively recommended value. ± = estimated uncertainty of recommended value.

## VI. BIBLIOGRAPHY

- 51A R.A. Alberty, R.M. Smith, and R.M. Bock, *J. Biol. Chem.*, **1951**, *193*, 425  
53D V. Di Stefano and W.F. Neuman, *J. Biol. Chem.*, **1953**, *200*, 759  
54M N.C. Melchior, *J. Biol. Chem.*, **1954**, *208*, 615  
54S J. Schubert, *J. Amer. Chem. Soc.*, **1954**, *76*, 3442  
56B R.M. Bock, N.S. Ling, S.A. Morell, and S.H. Lipton, *Arch. Biochem. Biophys.*, **1956**, *62*, 253  
56M A.E. Martell and G. Schwarzenbach, *Helv. Chim. Acta*, **1956**, *37*, 653  
56S R.M. Smith and R.A. Alberty, *J. Phys. Chem.*, **1956**, *60*, 180  
56Sa R.M. Smith and R.A. Alberty, *J. Amer. Chem. Soc.*, **1956**, *78*, 2376  
57N L.B. Nanninga, *J. Phys. Chem.*, **1957**, *61*, 1144  
57S G. Schwarzenbach and G. Anderegg, *Helv. Chim. Acta*, **1957**, *40*, 1229  
58M N.C. Melchior and J.B. Melchior, *J. Biol. Chem.*, **1958**, *231*, 609  
58W E. Walaas, *Acta Chem. Scand.*, **1958**, *12*, 528; **1957**, *11*, 1082  
58Wa G. Weitzel and T. Spehr, *Z. Physiol. Chem.*, **1958**, *313*, 212  
59B K. Burton, *Biochem. J.*, **1959**, *71*, 388  
60B H. Brintzinger and S. Fallab, *Helv. Chim. Acta*, **1960**, *43*, 54  
60O J. Olivard, *Arch. Biochem. Biophys.*, **1960**, *88*, 382  
60R M. Rawitscher and J.M. Sturtevant, *J. Amer. Chem. Soc.*, **1960**, *82*, 3739  
61B H. Brintzinger, *Helv. Chim. Acta*, **1961**, *44*, 935, 1199  
61N L.B. Nanninga, *Biochim. Biophys. Acta*, **1961**, *54*, 330  
61T E.R. Tucci, E. Doody, and N.C. Li, *J. Phys. Chem.*, **1961**, *65*, 1570  
62A H. Asai and M. Morales, *Arch. Biochem. Biophys.*, **1962**, *99*, 383  
62C J.J. Christensen and R.M. Izatt, *J. Phys. Chem.*, **1962**, *66*, 1030  
62H U. Handschin and H. Brintzinger, *Helv. Chim. Acta*, **1962**, *45*, 1037  
62I R.M. Izatt and J.J. Christensen, *J. Phys. Chem.*, **1962**, *66*, 359  
62T M.M. Taqui Khan and A.E. Martell, *J. Phys. Chem.*, **1962**, *66*, 10  
62Ta M.M. Taqui Khan and A.E. Martell, *J. Amer. Chem. Soc.*, **1962**, *84*, 3037  
63G P. George, R.C. Phillips, and R.J. Rutman, *Biochem.*, **1963**, *2*, 508  
63P R.C. Phillips, P. George, and R.J. Rutman, *Biochem.*, **1963**, *2*, 501  
63S J. Stockx and L. Vandendriessche, *Biochim. Biophys. Acta*, **1963**, *72*, 137  
63W S. Watanabe, T. Trosper, M. Lynn, and L. Evenson, *J. Biochem. (Tokyo)*, **1963**, *54*, 17; *Chem. Abstr.*, **1964**, *60*, 12267h  
64H G.G. Hammes and S.A. Levison, *Biochem.*, **1964**, *3*, 1504  
64O W.J. O'Sullivan and D.D. Perrin, *Biochem.*, **1964**, *3*, 18; *Biochem. Biophys. Acta*, **1961**, *52*, 612  
64S H. Sigel and H. Brintzinger, *Helv. Chim. Acta*, **1964**, *47*, 1701  
64Sa P.W. Schneider, H. Brintzinger, and H. Erlenmeyer, *Helv. Chim. Acta*, **1964**, *47*, 992  
65A G. Anderegg, *Helv. Chim. Acta*, **1965**, *48*, 1712  
65B J. Botts, A. Chashin, and H.L. Young, *Biochem.*, **1965**, *4*, 1788  
65P R. Phillips, P. Eisenberg, P. George, and R.J. Rutman, *J. Biol. Chem.*, **1965**, *240*, 4393  
66D E. Doody, E.R. Tucci, R. Scruggs, and N.C. Li, *J. Inorg. Nucl. Chem.*, **1966**, *28*, 833  
66I A.R. Irani and T.A. Tauli, *J. Inorg. Nucl. Chem.*, **1966**, *28*, 1011  
66Ia R.M. Izatt, J.H. Rytting, L.D. Hansen, and J.J. Christensen, *J. Amer. Chem. Soc.*, **1966**, *88*, 2641  
66P R.C. Phillips, P. George, and R.J. Rutman, *J. Amer. Chem. Soc.*, **1966**, *88*, 2631  
66Pa D.D. Perrin and V.S. Sharma, *Biochim. Biophys. Acta*, **1966**, *127*, 35  
66T M.M. Taqui Khan and A.E. Martell, *J. Amer. Chem. Soc.*, **1966**, *88*, 668  
67A N.N. Aylward, *J. Chem. Soc. B*, **1967**, 401  
67C J.J. Christensen, J.H. Rytting, and R.M. Izatt, *J. Phys. Chem.*, **1967**, *71*, 2700  
67S H. Sigel, K. Becker, and D.B. McCormick, *Biochim. Biophys. Acta*, **1967**, *148*, 655  
67T M.M. Taqui Khan and A.E. Martell, *J. Amer. Chem. Soc.*, **1967**, *89*, 5585  
68N G. Noat, J. Ricard, M. Borel, and C. Got, *Eur. J. Biochem.*, **1968**, *5*, 55  
68R C. Ropars, M. Rougee, M. Momenteau, and D. Lexa, *J. Chim. Phys.*, **1968**, *65*, 823  
68S H. Sigel, *Eur. J. Biochem.*, **1968**, *3*, 530  
69B J.P. Belaich and J.C. Sari, *Proc. Nat. Acad. Sci.*, **1969**, *64*, 763  
70B J.M. Blair, *Eur. J. Biochem.*, **1970**, *13*, 384  
70C J.J. Christensen, J.H. Rytting, and R.M. Izatt, *Biochem.*, **1970**, *9*, 4907  
70J J.M. Jallon and M. Cohn, *Biochim. Biophys. Acta*, **1970**, *222*, 542  
70M M.S. Mohan and G.A. Rechnitz, *J. Amer. Chem. Soc.*, **1970**, *92*, 5839; *Science*, **1970**, *168*, 1460; (see also N.C. Melchior, *Science*, **1971**, *171*, 1267)  
70N J.G. Norby, *Acta Chem. Scand.*, **1970**, *24*, 3276  
70Na G. Noat, J. Ricard, M. Borel, and C. Got, *Eur. J. Biochem.*, **1970**, *13*, 347  
70W A. Wrobel, A. Rabczenko, and D. Shugar, *Acta Biochim. Pol.*, **1970**, *17*, 339  
71B H.F. Bunn, B.J. Ransil, and A. Chao, *J. Biol. Chem.*, **1971**, *246*, 5273  
71I R.M. Izatt, J.J. Christensen, and J.H. Rytting, *Chem. Rev.*, **1971**, *71*, 439



- 71K E.E. Kriss and K.B. Yatsimirskii, *Russ. J. Inorg. Chem.*, **1971**, *16*, 202; *Zh. Neorg. Khim.*, **1971**, *16*, 386
- 71M J.P. Manners, K.G. Morallee, and R.J.P. Williams, *J. Inorg. Nucl. Chem.*, **1971**, *33*, 2085
- 71Ma O. Mäkitie and S. Mirttinen, *Suomen Kem.*, **1971**, *B44*, 155
- 71R K.S. Rajan, J.M. Davis, and R.W. Colburn, *J. Neurochem.*, **1971**, *18*, 345
- 72F C.M. Frey and J.E. Stuehr, *J. Amer. Chem. Soc.*, **1972**, *94*, 8898
- 72Fa C.M. Frey, J.L. Banyasz, and J.E. Stuehr, *J. Amer. Chem. Soc.*, **1972**, *94*, 9198
- 72M M.S. Mohan and G.A. Rechnitz, *J. Amer. Chem. Soc.*, **1972**, *94*, 1714
- 72S T. Sugano, T. Kitagawa, Y. Tsuda, T. Shibutani, and K. Kubo, *Nippon Kagaku Kaishi*, **1972**, *93*, 734
- 72T M.M. Taqui Khan and P.R. Reddy, *J. Inorg. Nucl. Chem.*, **1972**, *34*, 967
- 73B J.L. Banyase and J.E. Stuehr, *J. Amer. Chem. Soc.*, **1973**, *95*, 7226
- 73Ba H. Berger, G.R. Janig, G. Gerber, K. Ruckpaul, and S.M. Rapoport, *Eur. J. Biochem.*, **1973**, *38*, 553
- 73L P. Laget, P. Jallet, J. Wafflard, M. Moreau, H. Guerin, and J. Pieri, *J. Chim. Phys.*, **1973**, *70*, 1285
- 73S J.C. Sari and J.P. Belaich, *J. Amer. Chem. Soc.*, **1973**, *95*, 7491
- 73Sa J.C. Sari, M. Ragot, and J.P. Belaich, *Biochim. Biophys. Acta*, **1973**, *305*, 1
- 73T M.M. Taqui Khan and P.R. Reddy, *J. Inorg. Nucl. Chem.*, **1973**, *35*, 2813
- 73V K.M. Valentine and G.L. Cottam, *Arch. Biochem. Biophys.*, **1973**, *158*, 346
- 74B J.L. Banyasz and J.E. Stuehr, *J. Amer. Chem. Soc.*, **1974**, *96*, 6481
- 74E K.J. Ellis and J.F. Morrison, *Biochim. Biophys. Acta*, **1974**, *362*, 201
- 74F E.J. Fogt and G.A. Rechnitz, *Arch. Biochem. Biophys.*, **1974**, *165*, 604
- 74M M.S. Mohan and G.A. Rechnitz, *Arch. Biochem. Biophys.*, **1974**, *162*, 194
- 75B T.N. Briggs and J.E. Stuehr, *Anal. Chem.*, **1975**, *47*, 1916
- 75K I.V. Kolosov, *Soviet J. Coord. Chem.*, **1975**, *1*, 282; *Koord. Khim.*, **1975**, *1*, 357
- 75S H. Sigel, *J. Amer. Chem. Soc.*, **1975**, *97*, 3209
- 75T M.M. Taqui Khan and P.R. Reddy, *J. Inorg. Nucl. Chem.*, **1975**, *37*, 771
- 76K P.K. Kobos and G.A. Rechnitz, *Arch. Biochem. Biophys.*, **1976**, *175*, 11
- 76O N. Ogasawara and Y. Inoue, *J. Amer. Chem. Soc.*, **1976**, *98*, 7048
- 76R K.S. Rajan, A.A. Manian, J.M. Davis, and H. Dekirmenjian, *Brain Res.*, **1976**, *107*, 317
- 76S R.M. Smith and A.E. Martell, *Critical Stability Constants*, Volume 2, Amine Complexes, Plenum Publ. Co., New York, **1976**
- 76T M.M. Taqui Khan and P.R. Reddy, *J. Inorg. Nucl. Chem.*, **1976**, *38*, 1234
- 76Ta R.S. Taylor and H. Diebler, *Bioinorg. Chem.*, **1976**, *6*, 247
- 77C P. Chandhuri and H. Sigel, *J. Amer. Chem. Soc.*, **1977**, *99*, 3142
- 77N C. Nakai and W. Glinsmann, *Biochem.*, **1977**, *16*, 5636
- 77P A. Peguy and H. Diebler, *J. Phys. Chem.*, **1977**, *81*, 1355
- 77R M. Ragot, J.C. Sari, and J.P. Belaich, *Biochim. Biophys. Acta*, **1977**, *499*, 411, 421
- 77S H. Sigel, *J. Inorg. Nucl. Chem.*, **1977**, *39*, 1903
- 77Sa H. Sigel, B.E. Fischer, and B. Puijs, *J. Amer. Chem. Soc.*, **1977**, *99*, 4489
- 78A R. Adolfsen and E.N. Moudrianakis, *J. Biol. Chem.*, **1978**, *253*, 4378
- 78D N.K. Davidenko, P.A. Manorik, and K.B. Yatsimirskii, *Russ. J. Inorg. Chem.*, **1978**, *23*, 1794; *Zh. Neorg. Khim.*, **1978**, *23*, 3233
- 78F Y. Fukuda, P.R. Mitchell, and H. Sigel, *Helv. Chim. Acta*, **1978**, *61*, 638
- 78G J. Galea, R. Beccaria, G. Ferroni, and J.P. Belaich, *Electrochim. Acta*, **1978**, *23*, 647
- 78Ga J. Galea, R. Beccaria, G. Ferroni, and J.P. Belaich, *Electrochim. Acta*, **1978**, *23*, 103
- 78Gb R.K. Gupta and J.L. Benovic, *Biochem. Biophys. Res. Comm.*, **1978**, *84*, 130
- 78K I.V. Kolosov, *Soviet J. Coord. Chem.*, **1978**, *4*, 397; *Koord. Khim.*, **1978**, *4*, 531
- 78M P.R. Mitchell and H. Sigel, *J. Amer. Chem. Soc.*, **1978**, *100*, 1564
- 78R K.S. Rajan, S. Mainer, and J.M. Davis, *Bioinorg. Chem.*, **1978**, *9*, 187
- 79B B.A. Bulos and B. Sacktor, *Anal. Biochem.*, **1979**, *95*, 62
- 79M M.R. Melardi, J. Galea, G. Ferroni, A. Belaich, and M. Ragot, *Bull. Soc. Chim. Belg.*, **1979**, *88*, 1015
- 79Ma S. Murao, M. Kameda, and T. Nishina, *Agric. Biol. Chem.*, **1979**, *43*, 1795
- 79Mb H.C. Malhotra and L.K. Sharma, *Gazz. Chim. Ital.*, **1979**, *109*, 113
- 79Mc M.S. Mohan and M.M. Taqui Khan, *J. Coord. Chem.*, **1979**, *8*, 207
- 79T H.H. Trimm and R.C. Patel, *Inorg. Chim. Acta*, **1979**, *35*, 15
- 80D N.K. Davidenko and P.A. Manorik, *Russ. J. Inorg. Chem.*, **1980**, *25*, 239; *Zh. Neorg. Khim.*, **1980**, *25*, 437
- 80Da N.K. Davidenko and P.A. Manorik, *Russ. J. Inorg. Chem.*, **1980**, *25*, 247; *Zh. Neorg. Khim.*, **1980**, *25*, 454
- 80Db N.K. Davidenko, P.A. Manorik, and K.B. Yatsimirskii, *Russ. J. Inorg. Chem.*, **1980**, *25*, 491; *Zh. Neorg. Khim.*, **1980**, *25*, 883
- 80K R. Kramer, *Biochim. Biophys. Acta*, **1980**, *592*, 615
- 80M M.R. Melardi, J. Galea, G. Ferroni, A. Belaich, and M. Ragot, *Electrochim. Acta*, **1980**, *25*, 1007
- 80Ma J.F. Morrison and W.W. Cleland, *Biochem.*, **1980**, *19*, 3127
- 80O J.B. Orenberg, B.E. Fischer, and H. Sigel, *J. Inorg. Nucl. Chem.*, **1980**, *42*, 785
- 80R F. Ramirez, J.F. Marecek, and J. Szamosi, *J. Org. Chem.*, **1980**, *45*, 4748
- 80T J.C. Thomas, C.M. Frey, and J.E. Stuehr, *Inorg. Chem.*, **1980**, *19*, 501
- 80Ta J.C. Thomas, C.M. Frey, and J.E. Stuehr, *Inorg. Chem.*, **1980**, *19*, 505

- 80Tb J. Tummavuori and S. Suntioinen, *Finn. Chem. Lett.*, **1980**, 113.  
80V R.E. Viola, J.F. Morrison, and W.W. Cleland, *Biochem.*, **1980**, *19*, 3131  
81B E.O. Bishop, S.J. Kimber, D. Orchard, and B.E. Smith, *Biochim. Biophys. Acta*, **1981**, *635*, 63  
81C R. Cali, S. Musumeci, C. Rigano, and S. Sammartano, *Inorg. Chim. Acta*, **1981**, *56*, L11  
81M A.E. Martell and R.M. Smith, *Critical Stability Constants*, Volume 5, First Supplement, Plenum Publ. Co., New York, **1981**  
81N A. Nagasawa and H. Diebler, *J. Phys. Chem.*, **1981**, *85*, 3523  
81W S.T. Wu, G.M. Pieper, J.M. Salhany, and R.S. Eliot, *Biochem.*, **1981**, *20*, 7399  
82S J.C. Sari, M. Hadida, A.M. Chauvet-Monges, and A. Crevat, *J. Bioenerg. Biomembr.*, **1982**, *14*, 171  
82Sa S.M. Shanbhag, Ph.D. Diss., Florida State Univ., **1982**  
82V W.H. Voige and R.I. Elliott, *J. Chem. Educ.*, **1982**, *59*, 257  
83A G. Arena, R. Cali, V. Cucinotta, S. Musumeci, E. Rizzarelli, and S. Sammartano, *J. Chem. Soc. Dalton*, **1983**, 1271  
83C A. Cole, P.M. May, and D.R. Williams, *Agents Actions*, **1983**, *13*, 91  
83Ca L.G. Clary, W.H. Voige, and J.J. Leary, *Anal. Biochem.*, **1983**, *129*, 228  
83G J.L. Gabriel, T. Aogaichi, C.R. Dearolf, and G.W.E. Plaut, *Anal. Lett.*, **1983**, *16*, 113  
83J G.E. Jackson and M.J. Kelly, *Polyhedron*, **1983**, *2*, 1313  
83M J.F. Morrison and W.W. Cleland, *Biochem.*, **1983**, *22*, 5507  
83R P.R. Reddy, K.V. Reddy, and M.M. Taqui Khan, *Indian J. Chem.*, **1983**, *22A*, 959  
83S S.G. Sysieva, E.Z. Utyanskaya, and M.I. Vinnik, *Bull. Acad. Sci. USSR, Ser. Chem.*, **1983**, *32*, 1364; *Izv. Akad. Nauk S.S.R., Ser. Khim.*, **1983**, *32*, 1505  
83W E.R. Werner and B.M. Rode, *Inorg. Chim. Acta*, **1983**, *80*, 39  
84C G. Crisponi, R. Caminiti, S. Biagini, M. Casu, and A. Lai, *Polyhedron*, **1984**, *3*, 1105  
84E C.D. Eads, P. Mulqueen, W.D. Horrocks, Jr., and J.J. Villafranka, *J. Biol. Chem.*, **1984**, *259*, 9379  
84G A.S. Grigoreva, N.F. Konakhovich, L.I. Budarin, and F.P. Trinus, *Soviet J. Coord. Chem.*, **1984**, *10*, 815; *Koord. Khim.*, **1984**, *10*, 1460  
84J W.T. Jenkins, M.M. Marshall, and A.S. Lewin, *Arch. Biochem. Biophys.*, **1984**, *232*, 496  
84M P.A. Manorik, N.K. Davidenko, N.P. Aleksyuk, and E.I. Lopatina, *Russ. J. Inorg. Chem.*, **1984**, *29*, 424; *Zh. Neorg. Khim.*, **1984**, *29*, 735  
84P V.L. Pecoraro, J.D. Hermes, and W.W. Cleland, *Biochem.*, **1984**, *23*, 5262  
84S H. Sigel and K.H. Scheller, *Eur. J. Biochem.*, **1984**, *138*, 291  
84Sa H. Sigel, K.H. Scheller, and R.M. Milburn, *Inorg. Chem.*, **1984**, *23*, 1933  
85B S. Biagini, M. Casu, A. Lai, R. Caminiti, and G. Crisponi, *Chem. Phys.*, **1985**, *93*, 461  
85J W.T. Jenkins, *Anal. Biochem.*, **1985**, *145*, 362  
85K C.R. Krishnamoorthy, S. Sunil, and K. Ramalingam, *Polyhedron*, **1985**, *4*, 1451  
85M K. Matsuda, C. Kanai, M. Takahara, and M. Maki, *Nippon Kagaku Kaishi*, **1985**, 698  
85O E.I. Ochiai and R. Morand, *J. Coord. Chem.*, **1985**, *14*, 83  
85T R. Tribolet, R. Malini-Balakrishnan, and H. Sigel, *J. Chem. Soc. Dalton*, **1985**, 2291  
86C R. Cini, A. Cinquantini, and R. Seeber, *Inorg. Chim. Acta*, **1986**, *123*, 69  
86D A. De Robertis, C. De Stefano, S. Sammartano, R. Cali, R. Purrello, and C. Rigano, *J. Chem. Res. (S)*, **1986**, 164; *J. Chem. Res. (M)*, **1986**, 1301  
87H M.J. Hynes and M. O'Dowd, *J. Chem. Soc. Dalton*, **1987**, 563  
87J G.E. Jackson and K.V. Vovi, *Polyhedron*, **1987**, *6*, 2095  
87S H. Sigel, R. Tribolet, R. Malini-Balakrishnan, and R.B. Martin, *Inorg. Chem.*, **1987**, *26*, 2149  
87Sa S.M. Shanbhag and G.R. Choppin, *Inorg. Chim. Acta*, **1987**, *138*, 187  
87Sb S.M. Shanbhag and G.R. Choppin, *Inorg. Chim. Acta*, **1987**, *139*, 119  
87Sc I.E. Svetlova, N.S. Smirnova, N.A. Dobrynina, L.I. Martynenko, A.M. Evseev, and V.I. Spitsyn, *Dokl. Chem.*, **1987**, *294*, 266; *Dokl. Akad. Nauk SSSR*, **1987**, *294*, 890  
87T R. Tribolet and H. Sigel, *Eur. J. Biochem.*, **1987**, *163*, 353  
88A M.L. Antonelli, S. Balzamo, V. Carunchio, E. Cernia, and R. Purrello, *J. Inorg. Biochem.*, **1988**, *32*, 153  
88B A. Bianchi, M. Micheloni, and P. Paoletti, *Inorg. Chim. Acta*, **1988**, *151*, 269  
88G A. Gianguzza, G. Dia, S. Sammartano, and C. De Stefano, *J. Chem. Res. (S)*, **1988**, 12; *J. Chem. Res. (M)*, **1988**, 369  
88M S.S. Massoud and H. Sigel, *Inorg. Chem.*, **1988**, *27*, 1447  
88Ma S.S. Massoud and H. Sigel, *Bull. Chem. Soc. Ethiop.*, **1988**, *2*, 9  
88R M.V. Rekharsii, S.A. Tishchenko, A.M. Egorov, and G.L. Galchenko, *Moscow Univ. Chem. Bull.*, **1988**, *43*, No. 1, 52; *Vestnik Mosk. Univ., Khim.*, **1988**, *43*, 46  
88S I.E. Svetlova, N.S. Smirnova, N.A. Dobrynina, L.I. Martynenko, and A.M. Evseev, *Russ. J. Inorg. Chem.*, **1988**, *33*, 643; *Zh. Neorg. Khim.*, **1988**, *33*, 1135  
88Sa H. Sigel, S.S. Massoud, and R. Tribolet, *J. Amer. Chem. Soc.*, **1988**, *110*, 6857  
88T R. Tribolet and H. Sigel, *Eur. J. Biochem.*, **1988**, *170*, 617  
89M S.S. Massoud and H. Sigel, *Eur. J. Biochem.*, **1989**, *179*, 451  
89S R.M. Smith and A.E. Martell, *Critical Stability Constants*, Volume 6, Second Supplement, Plenum Publ. Co., New York, **1989**