NATIONAL BUREAU OF STANDARDS REPORT

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TENTH PRELIMINARY REPORT ON
A SURVEY OF THERMODYNAMIC PROPERTIES OF THE
COMPOUNDS OF THE ELEMENTS CHNOPS

Progress Report for the Period 1 October to 31 December 1966

to

National Aeronautics and Space Administration

1 March 1967

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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A SURVEY OF THERMODYNAMIC PROPERTIES OF THE

COMPOUNDS OF THE ELEMENTS CHNOPS

George T. Furukawa, Martin L. Reilly

Gerald D. Mitchell, George T. Armstrong

Heat Division, Institute for Basic Standards

Progress Report for the Period 1 October to 31 December 1966

to

National Aeronautics and Space Administration

Contract No. R-138, Amendment 2.

<NBS>

U. S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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FOREWORD

        A study at the National Bureau of Standards (NBS), of which
this is the tenth progress report, has been undertaken to meet
the need of the National Aeronautics and Space Administration (NASA)
for thermodynamic information on biologically related materials
important to the space program for several reasons. Among these
reasons are the necessity of inferring the maximum amount of useful
chemistry of incompletely accessible environments, for which only
limited information is available, the possibility of the occurrence
of organic compounds naturally synthesized under primitive condi-
tions, and the possibility of theoretically recovering part of the
prebiological history of the earth.

        This program is being carried out under the technical super-
vision of Dr. George Jacobs of NASA, and with the consultation of
Dr. Harold Morowitz of the Yale University, Department of Molecular
Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division,
Institute for Basic Standards (NBS). The contract (Contract No. R-138)
was initiated 1 May 1964 and extended 29 April 1965. The program has
been extended by Amendments 1 and 2. This report covers the first
quarter of the work being carried out under Amendment 2.

                            _____
                            George P. Armstrong
                            Supervisory Chemist
                            Project Leader

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Section I

Analysis of Heat-Capacity and Vapor-Pressure Data

George T. Furukawa and Martin L. Reilly

The analysis of heat-capacity data has been directed largely on the higher molecular weight C-H compounds. Intensive examination of the data showed inconsistencies in the published analyses of the observations in the "premelting" region for some of the substances. A new computer method was developed to perform an improved analysis of the data in this temperature range.

The compilation of vapor-pressure data is new to the group. There was, therefore, no immediate source of vapor-pressure data to carry out the analysis. An effort was started to compile vapor-pressure data on the same relatively high molecular weight C-H compounds for which the heat-capacity data were available. The existing compilations, such as those by Timmermans, Stull, etc., were consulted. A computer code for analyzing the vapor-pressure data is being developed.

The following is the list of C-H compounds on which the analysis of heat-capacity data is in various stages of completion and for which the vapor-pressure data are being compiled:

A. normal paraffins: C_9, C_{10}, C_{11}, C_{12}, C_{13}, C_{14}, C_{15}, C_{16}, C_{32}, and C_{36}.

B. aromatic hydrocarbons: benzene, naphthalene, anthracene, phenanthrene, pyrene, 1-methylnaphthalene, and 2-methylnaphthalene.

C. others: tetralin, cis-decalin, trans-decalin, and adamantane.

The relatively old heat-capacity data on alloxan, allantoin, uric acid, xanthine, guanine, hypoxanthine, and lactic acid for which measurements extend down only to about 80°K have been re-examined to obtain a better extrapolation to 0°K. Further efforts are still needed at this time to reduce the uncertainty of the extrapolation.

Section II

Gibbs Energies, Entropies and Enthalpies of Solution, Dilution, and Formation of Selected Ubiquitous Compounds

Gerald D. Mitchell and George T. Armstrong

A selected list of amino acids, purine and pyrimidine bases, sugars, fatty acids, glycerol, was the basis of a search for additional thermodynamic data beyond that published in our previous reports. The heat, entropy, and Gibbs energy of formation in the free state, the enthalpies, entropies and Gibbs energies of solution, the enthalpies of dilution and the Gibbs energy of formation of the aqueous state were found for many but not all of these substances. A list of the compounds with a description of the data selected for each follows, including values from our previous work when they existed. The discussion gives a reference to the source of the data in the following list of references. Numerous gaps exist in the data.

Table 1.

Selected Thermodynamic Data

L-Alanine

$\underline{\Delta G^o_{298}, \Delta S^o_{298}}$

Gibbs energy and entropy of formation are given by Domalski [6]*
from data given in previous reports. $\Delta G^o_{298} = -87.94$ kcal mol^{-1};
$\Delta S^o_{298} = -154.34$ cal(deg mol)$^{-1}$.

$\underline{\Delta H^o_{298}}$

The heat of formation reported in [6] was taken from Table 1,
NBS Report 8641, p. 12 [7].

$\underline{\Delta H_{298}(\text{solution})}$

The heat of solution as determined calorimetrically by Zittle is
$\Delta H_{298} = 2140 \pm 30$ cal mol^{-1} [12].

$\underline{\Delta H_{298}(\text{dilution})}$

The heat of dilution as determined directly by Zittle is
$\Delta H_{298} = 210$ cal mol^{-1} [12].

$\underline{\Delta G_{298}(\text{in solution})}$

Krebs and Kornberg [5] list Burton and Krebs [14] value for
ΔG_{298} of formation in solution, -88.75 kcal mol^{-1}.

$\underline{\Delta G_{298}(\text{of solution})}$

The Gibbs energy of solution of L-alanine is given in [13] by
Greenstein. $\Delta G_s = -350$ cal mol^{-1}.

$\underline{\Delta S_{298}(\text{of solution})}$

Calculated from existing data, ΔG_s [13] and ΔH_s [9],
$\Delta S^o_{298} = 8.0161$ cal(deg mol)$^{-1}$.

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* Figures in brackets indicate literature references listed at
end of this chapter.

ℓ-Arginine

ΔH^{O}_{298}

Domalski and Halow [7] list Huffman, Fox, and Ellis [15] value of the heat of formation ΔH^{O}_{298} = -148.66 kcal mol^{-1}.

ΔG^{O}_{298}

Gibbs energy of formation of pure substance is given by Krebs and Kornberg [5], taken from Huffman and Ellis [16], ΔG^{O}_{298} = 57.44 kcal mol^{-1}.

ΔS^{O}_{298}

Data calculated from ΔH^{O}_{298} and ΔG^{O}_{298} given in [7] and [5] respectively, ΔS^{O}_{298} = -305.95 cal(deg mol)$^{-1}$.

ΔH_{298}(of solution)

The heat of solution of ℓ-arginine, ΔH_{298} = 1500 cal mol^{-1}, is given by Zittle and Schmidt [12].

ℓ-Aspartic Acid

ΔH^{O}_{298}, ΔS^{O}_{298}, ΔG^{O}_{298}

Data taken from [6] as given by Domalski, ΔH^{O}_{298} = -232.47 kcal mol^{-1}, ΔS^{O}_{298} = -194.94 cal(deg mol)$^{-1}$, ΔG^{O}_{298} = -174.35 kcal mol^{-1}.

ΔH_{298}(of solution)

Data obtained by direct measurement is given by Zittle and Schmidt [12]. ΔH_{298} = 6000 cal mol^{-1}.

ΔG_{298}(in solution)

Krebs and Kornberg [5] report the value of Burton and Krebs [14]. ΔG_{f298} = 172.31 kcal mol^{-1}.

ΔG_{298}(of solution)

Greenstein [13] reports ΔG_{S} to be +2550 cal mol^{-1}.

ΔS_{298}(solution)

Calculated from ΔH_{S} and ΔG_{S} given in [12] and [13], respectively. ΔS_{298} = 11.5714 cal(deg mol)$^{-1}$.

L-Asparagine·H_2O

ΔH^o_{298}, ΔS^o_{298}, ΔG^o_{298}

Heat, Gibbs energy, and entropy of formation. Data from Domalski [6]. ΔH^o_{298} = -259.52 kcal mol^{-1}, ΔS^o_{298} = -255.19 cal(deg mol)$^{-1}$, ΔG^o_{298} = -183.44 kcal mol^{-1}.

ΔH_{298}(of solution)

The experimental value as determined by Dalton and Schmidt [8] is ΔH_{298} = 8000 cal mol^{-1}.

ΔG_{298}(in solution)

Krebs and Kornberg [5] report Barsook and Huffman [18] value, ΔG_{298} = -125.86 kcal mol^{-1}.

ΔG_{298}(of solution)

Greenstein [13] reports the value of +950 cal mol^{-1} for the Gibbs energy of solution.

ΔS_{298}(of solution)

We calculated ΔS = 23.6458 cal(deg mol)$^{-1}$ from data in [8] and [13], ΔH, ΔG respectively.

Cysteine

ΔG^o_{298} (pure compound)

Krebs and Kornberg [5] report values calculated from Borsook, Ellis and Huffman [17], ΔG^o_{298} = -163.55 kcal mol^{-1}.

ΔG^o_{298}(in solution)

ΔG^o_{298} = -159.00 listed by Krebs and Kornberg [5], calculated from Borsook, Ellis and Huffman [17].

Glutamic Acid

ΔH^O_{298}, ΔS^O_{298}, ΔG^O_{298}

Data reported by Domalski [6]. ΔH^O_{298} = -240.05 kcal mol^{-1}; ΔS^O_{298} = -223.19 cal(deg mol)$^{-1}$; ΔG^O_{298} = -173.51 kcal mol^{-1}.

ΔH_{298}(solution)

Zittle and Schmidt [12] report a value for the heat of solution, ΔH_S = 6530 cal mol^{-1}.

ΔG_{298}(in solution)

Krebs and Kornberg [5] report Borsook and Huffman's [18] data for the Gibbs energy of formation in aq. solution, ΔG_{298} = -171.75 kcal mol^{-1}.

ΔG_{298}(of solution)

The value for the Gibbs energy of solution is given in [13] by Greenstein. ΔG_S = 2300 kcal mol^{-1}.

ΔS^O_{298}(of solution)

Calculated from data in [12] and [13], ΔS^O_S = 14.1875 cal(deg mol)$^{-1}$.

Glutamine

ΔH^O_{298}, ΔS^O_{298}, ΔG^O_{298}

Data given by Domalski [6] is taken from previous reports. ΔH^O_{298} = -197.8 kcal mol^{-1}, ΔS^O_{298} = -235.53 cal(deg mol)$^{-1}$, ΔG^O_{298} = -127.60 kcal mol^{-1}.

Glycine

ΔH^O_{298}, ΔS^O_{298}, ΔG^O_{298}

The value given by Domalski [6] is taken from previous reports. ΔH = -126.22 kcal mol^{-1}, ΔS^O_{298} = -127.88 cal(deg mol)$^{-1}$, ΔG^O_{298} = -88.09 kcal mol^{-1}.

ΔH_{298}(of solution)

Zittle and Schmidt [12] report a value of 3750 cal mol^{-1}.

ΔH_{298}(of dilution)

Zittle and Schmidt [12] give an experimental value of 225 cal mol^{-1}.

ΔG_{298}(in solution)

Reported by Krebs and Kornberg [5], taken from Rossini et al. [19], ΔG_{298} = -89.26 kcal mol^{-1}.

ΔG_{298}(of solution)

Greenstein and Winitz [13] give the Gibbs energy of solution as -650 cal mol^{-1}.

ΔS_{298}(of solution)

Calculated from data given in [12,13], ΔH_{298}, ΔG_{298} of solution. ΔS_{298} = 14.7577 cal(deg mol)$^{-1}$.

L-Histidine

ΔH (of solution)

Zittle and Schmidt [12] give a value of 3300 cal mol^{-1} for the heat of solution.

ΔH_{298}(dilution)

Greenstein and Winitz [13] give -90 cal mol^{-1} as the heat of dilution.

ℓ-Isoleucine

ΔH_{298}^{o}, ΔG_{298}^{o}, ΔS_{298}^{o}

Domalski in [6] gives the values ΔH_{298}^{o} = -151.8 kcal mol^{-1}, ΔS_{298}^{o} = -233.33 cal(deg mol)$^{-1}$, ΔG_{298}^{o} = -82.2 kcal mol^{-1}.

ΔH^{o} (of solution)

Dalton and Schmidt [8] report a calculated value of 843 cal mol^{-1}.

ΔG (of solution)

Greenstein and Winitz [13] report 700 cal mol^{-1} for the Gibbs energy of solution.

ΔS (of solution)

Calculated from the data given in [8] and [13], ΔH_s and ΔG_s give ΔS_{298} = 0.4796 cal(deg mol)$^{-1}$.

Leucine

ΔH^o_{298}, ΔS^o_{298}, ΔG^o_{298}

Domalski in reference [6] reports the values ΔH^o_{298} = -151.97 kcal mol^{-1}, ΔS^o_{298} = -232.37 cal(deg mol)$^{-1}$, and ΔG^o_{298} = -82.68 kcal mol^{-1}.

ΔG^o_{298} (in solution)

Krebs and Kornberg [5] report Borsook and Huffman's [18] value adjusted (+0.03 Kg cal) for ΔG^o of racemization. ΔG^o_{298} = -81.68 kcal mol^{-1}.

ΔG_{298} (of solution)

Greenstein and Winitz [13] give the value of 950 cal mol^{-1}.

ΔH_{298} (of solution)

Dalton and Schmidt [9] report ΔH_{298} = 830 cal mol^{-1} corrected for activity of amino acid.

ΔS_{298} (of solution)

Calculated from ΔG_{298} and ΔH_{298} of solutions [13], [9]. ΔS_{298} = -0.4025 cal(deg mol)$^{-1}$.

Lysine

ΔH^o_{298}

Domalski and Halow [7] report Ponomarev and Migarskaya [20] value ΔH^o_{298} = -162.2 kcal mol^{-1}.

ΔH_{298} (of solution)

Zittle and Schmidt [12] give a value of 4000 ±100 cal mol^{-1}.

ΔH_{298} (of dilution)

Greenstein and Winitz [13] give ΔH_{298} of dilution to be 500 cal mol^{-1}.

ℓ-Methionine

ΔH^o_{298}

Domalski and Halow [7] report Tsuzuki, Harper, and Hunt's [21] value -180.4 kcal mol^{-1}.

ΔS^o_{298}

Hutchens, Cole, and Stout [10] report the entropy as calculated from the elements [19].

ΔH_{298}(of solution)

Dalton and Schmidt [8] give an experimental value of 4100 cal mol^{-1}.

ΔG_{298}(of solution)

Greenstein and Winitz [13] give 850 cal mol^{-1} for the Gibbs energy of solution.

ΔS_{298}(of solution)

Calculated from the data in [8], [13], ΔG_{298} and ΔH_{298} of solution. ΔS_{298} = 10.5652 cal(deg mol)$^{-1}$.

ℓ-Phenylalanine

ΔH^o_{298}, ΔS^o_{298}, ΔG^o_{298}

Domalski [6] reports the values ΔH^o_{298}=-111.9 kcal mol^{-1}, ΔS^o_{298} = -204.87 cal(deg mol)$^{-1}$ and ΔG^o_{298} = -50.6 kcal mol^{-1}.

ΔH_{298}(of solution)

Dalton and Schmidt [9] give the corrected value of 2770 cal mol^{-1} for the heat of solution.

ΔG^o_{298}(of solution)

Greenstein and Winitz [13] report 1000 cal mol^{-1} for the Gibbs energy of solution.

ΔS^o_{298}(of solution)

Calculated from the data in [9,13], ΔH_{298} and ΔG_{298} of solution. ΔS_{298} = 5.9366 cal(deg mol)$^{-1}$.

Proline

ΔH^O_{298}, ΔS^O_{298}, ΔG^O_{298}

Domalski [6] reported the values $\Delta H^O_{298} = -125.7$ kcal mol^{-1}, $\Delta S^O_{298} = -179.97$ cal(deg mol)$^{-1}$, $\Delta G^O_{298} = -72.0$ kcal mol^{-1}.

ΔH_{298} (of solution)

Greenstein and Winitz [13] report 750 cal mol^{-1} for the heat of solution.

ΔH_{298} (dilution)

Greenstein and Winitz [13] give an experimental value of 1050 cal mol^{-1}.

ΔG_{298} (of solution)

Greenstein and Winitz [13] reports -1450 cal mol^{-1}.

ΔS_{298} (of solution)

Calculated from data in [13], ΔG_{298} and ΔH_{298} of solution. $\Delta S_{298} = 7.3788$ cal(deg mol)$^{-1}$.

Serine

ΔH^O_{298}, ΔS^O_{298}, ΔG^O_{298}

Hutchins, Cole, and Stout [11] give experimental values of $\Delta H^O_{298} = -173.6$ kcal mol^{-1}, $\Delta S^O_{298} = -174.06$ cal(deg mol)$^{-1}$, and $\Delta G^O_{298} = -121.6$ kcal mol^{-1}.

ΔH_{298}, ΔG_{298} (of solution)

Greenstein and Winitz [13] report $\Delta H_{298} = 5180$ cal mol^{-1} and $\Delta G_{298} = 450$ cal mol^{-1} of solution.

ΔS_{298} (of solution)

Calculated from data in [13], ΔS is 15.8645 cal(deg mol)$^{-1}$.

ΔH_{298} (dilution)

Greenstein and Winitz's [13] experimental value is -130 cal mol^{-1}.

Threonine

ΔH^{o}_{298}

Domalski and Halow [7] report Tsuzuki, Harper and Hunter's [21] value for the heat of formation. $\Delta H^{o}_{298} = -181.4$ kcal mol^{-1}.

ΔG_{298}(in solution)

Krebs and Kornberg [5] give Metzler, Langenecker, and Snell's [22] approximate value of -123.0 kcal mol^{-1}.

Tryptophane

ΔH^{o}_{298}, ΔS^{o}_{298}, ΔG^{o}_{298}

Domalski [6] gives the values $\Delta H^{o}_{298} = -99.8$ kcal mol^{-1}, $\Delta S^{o}_{298} = -237.29$ cal(deg mol)$^{-1}$, ΔG^{o}_{298} -29.1 kcal mol^{-1}.

ΔH_{298}(of solution)

Dalton and Schmidt [8] give a calculated value of 1300 cal mol^{-1} for the heat of solution.

ΔG_{298}(of solution)

Greenstein and Winitz [13] give a value of 1750 cal mol^{-1} for the Gibbs energy of solution.

ΔS_{298}(of solution)

Calculated from the data in [8,13], ΔG_{298}, ΔH_{298} of solution. $\Delta S_{298} = -1.3081$ cal(deg mol)$^{-1}$.

Tyrosine

ΔH^{o}_{298}, ΔS^{o}_{298}, ΔG^{o}_{298}

Domalski [6] reports a value of $\Delta H^{o}_{298} = -163.4$ kcal mol^{-1}, $\Delta S^{o}_{298} = -229.28$ cal(deg mol)$^{-1}$, $\Delta G^{o}_{298} = -95.06$ kcal mol^{-1}.

ΔG_{298}(in solution)

Krebs and Kornberg [5] report Huffman and Ellis' [16] value -92.55 kcal mol^{-1}.

ΔH_{298}(of solution)

Dalton and Schmidt [9] give a corrected value of 5960 cal mol^{-1} for the heat of solution.

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ΔG_{290}(of solution)

Greenstein and Winitz [13] report -3550 cal mol^{-1} for the Gibbs energy of solution.

ΔS_{298}(of solution)

Calculated from data in [9,13], ΔH_{298}, ΔG_{298} of solution. $\Delta S_{298} = 31.8967$ cal(deg mol)$^{-1}$.

Thymine

ΔH_{298}^{o}

Domalski [6] gives a value of -111.9 kcal mol^{-1}.

Valine

ΔH_{298}^{o}, ΔS_{298}^{o}, ΔG_{298}^{o}

Domalski [6] reports the values $\Delta H_{298}^{o} = -148.2$ kcal mol^{-1}, $\Delta S_{298}^{o} = -207.67$ cal(deg mol)$^{-1}$, $\Delta G_{298}^{o} = -86.3$ kcal mol^{-1}.

ΔG_{298}, ΔH_{298}(of solution)

Greenstein and Winitz [13] give the values $\Delta G_{298} = 350$ cal mol^{-1}, $\Delta H_{298} = 500$ cal mol^{-1}.

ΔS_{298}(of solution)

Calculated from the data given by Greenstein and Winitz [13], ΔG_{298} and ΔH_{298} of solution. $\Delta S_{298} = 0.503$ cal(deg mol)$^{-1}$.

D-Glucose

ΔH_{298}^{o}, ΔS_{298}^{o}, ΔG_{298}^{o}

Burton and Krebs [3] report values of $\Delta H_{298}^{o} = -304.64$ kcal mol^{-1}, $\Delta S_{298}^{o} = -291.7$ cal(deg mol)$^{-1}$ and $\Delta G_{298}^{o} = -217.56$ kcal mol^{-1}.

ΔG_{298}(in solution)

Burton and Krebs [3] report a value of -219.38 kcal mol^{-1}.

ΔG_{298}(of solution)

Burton and Krebs [3] give the value of -1820 cal mol^{-1}.

ΔH_{298}(of solution)

Taylor and Rowlinson [1] give a value of 2630 ± 10 cal mol^{-1}.

ΔS_{298}(of solution)

The value 14.9254 cal(deg mol)$^{-1}$ was calculated from data given by Burton and Krebs [26] and Taylor and Rowlinson [1].

ΔH_{298}(of dilution)

Lange and Markgraf [2] report an integral value of 28.55 ±0.16 cal mol^{-1} for a solution that is 0.3479 M.

Ribose

ΔH^{o}_{298}

Domalski and Halow [7] report a value of -253.9 kcal mol^{-1} for the heat of formation at 298.15°K.

Adenine

ΔH^{o}_{298}, ΔS^{o}_{298}, ΔG^{o}_{298}

Stiehler and Huffman [4] report a calculated value of -163.2 cal(deg mol)$^{-1}$ for ΔS^{o}_{298}, -70.420 kcal mol^{-1} for ΔG^{o}_{298} and -21.760 kcal mol^{-1} for ΔH^{o}_{298}.

Guanine

ΔH^{o}_{298}, ΔS^{o}_{298}, ΔG^{o}_{298}

Stiehler and Huffman [4] give calculated values, ΔH^{o}_{298} = -45.090 kcal mol^{-1}, ΔS^{o}_{298} = -185.6 cal(deg mol)$^{-1}$ and ΔG^{o}_{298} = 10.220 kcal mol^{-1}.

Butyric Acid

$\Delta H^O_{298}, \Delta S^O_{298}, \Delta G^O_{298}$

Burton and Krebs [3] report the values $\Delta H^O_{298} = -128.09$ kcal mol^{-1}, $\Delta S^O_{298} = -125.2$ cal(deg mol)$^{-1}$, $\Delta G^O_{298} = -90.65$ kcal mol^{-1}.

ΔG_{298}(in solution)

Burton and Krebs [3] give -91.2 kcal mol^{-1} for ΔG_{298} in aq. solution.

ΔG_{298}(of solution)

Burton and Krebs [3] report -550 cal mol^{-1} for the ΔG_{298} of solution.

Palmitic Acid

ΔG_{298}

Krebs and Kornberg [5] give Parks and Huffman's [3] value of -25.7 kcal mol^{-1} for the Gibbs energy of formation.

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