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NATIONAL BUREAU OF STANDARDS REPORT

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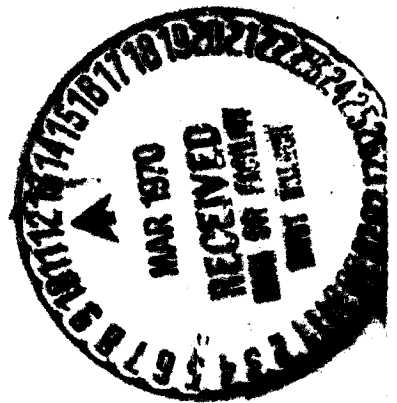
SEVENTEENTH REPORT ON A SURVEY OF THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

Progress Report for the Period 1 October through 31 December 1969

to

National Aeronautics and Space Administration
Contract No. ~~4-128~~, Admendment 4

W12-758



U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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George T. Armstrong and Eugene S. Domalski

Progress Report for the Period 1 October through 31 December 1969
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U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the seventeenth 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 conditions, and the possibility of theoretically recovering part of the pre-biological history of the earth.

This program is being carried out under the technical supervision 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 NBS. The contract (Contract No. R-138) was initiated 1 May 1964 and extended by Amendments 1, 2, 3, and 4. This report covers a portion of work under Amendment 4. A significant change in the direction of the project occurred with the initiation of Amendment 3. The work is now directed toward the presentation of the material in the form of a Handbook of Thermodynamic Data of Interest in the Biological Sciences. In this effort the work at NBS is coordinated with a related task at the Texas A and M Thermodynamic Properties Center under Dr. R. A. Wilhoit.

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Report of Progress

Prepared by George T. Armstrong

This Technical Report covers the principal progress made on the subject contract during the interval 1 October - 31 December 1970.

A meeting was held 6 November 1969 of R. C. Wilhoit, G. T. Furukawa, E. S. Domalski and George T. Armstrong at which the editorial plan of the handbook was laid out in detail. The information follows.

Plan of Publication of Handbook of Thermodynamic Properties of Biological Material.

1. As a result of the meeting the outline of the book as originally presented by Prof. Wilhoit is essentially unchanged except for the arrangement of chapters. Assignments were made for preparation of the chapters and the tables and a deadline was established, 21 March 1970, for first draft of all material to be in the editor's hands.

2. Wilhoit and Armstrong are to be joint editors. Individual chapters and tables will have joint authors and the principle contributors will be credited.

3. Chapter assignments are as follows:

Chapter 1 - Principles of Thermodynamics and Thermochemistry - Armstrong and Furukawa.

Chapter 2 - Thermodynamics of Solutions - Wilhoit.

Chapter 3 - Formulas and Computational Methods - Furukawa and Armstrong.

Chapter 4 - Methods of Calculating Equilibrium Composition of Multi-component Systems - Wilhoit.

Chapter 5 - Use of Thermodynamics in the Study of Living Organisms - Wilhoit.

Chapter 6 - Estimation of Thermodynamic Data - Domalski and Armstrong.

Chapter 7 - Review of Thermodynamic Data for Biologically Important Compounds - Domalski and Armstrong.

Chapter 8 - Glossary of Terms and Symbols, Units and Values of Fundamental Constants - Wilhoit.

4. Responsibility for Tables is as follows:

- Table 1 - Thermodynamic Functions of Temperatures - Furukawa.
- Table 2 - Thermodynamic Functions at 25°C - Domalski
- Table 3 - Heats of Combustion - Domalski.
- Table 4 - Vapor Pressure - Furukawa.
- Table 5 - Thermodynamic Functions of Solutions - Wilhoit.
- Table 6 - ΔG_f and ΔH_f of Aqueous Species not in Table 2 - Goldberg or Wilhoit.
- Table 7 - ΔG_f and ΔH_f of Aqueous Nucleotides not in Table 2 - Wilhoit.
- Table 8 - ΔG and ΔH for Some Reactions not Covered by Table 2 - Wilhoit.
- Table 9 - Solubilities in Water - Wilhoit.
- Table 10 - Physical Properties of Water and Some Aqueous Solutions -
- Table 11 - Properties of Some Buffer Solutions - Goldberg.
- Table 12 - Diffusion Coefficients -
- Table 13 - Soret Coefficients -

With regard to table 2 Wilhoit will supply appropriate data on solutions where required.

5. The tables are to be prepared sufficiently independently that each can stand alone, complete with tabular values, references, and a preliminary discussion which is judged by the author to be adequate to account for the values which are given. This preliminary discussion will be supplemented by Chapter 7 which will provide general information about the availability and quality of the data.

6. The bibliography and index arrangement were considered to be very important but best settled at a later date.

Substantial progress was made on the collection of selected heats of combustion and heats of formation of organic compounds. The material given on pages 4-37 of this report completes the material that is planned for compilation.

In reports of October 6, November 13, and December 8, 1969, the work being done by Dr. Wilhoit was summarized. A method of fitting observed thermodynamic data on two-component aqueous systems to parameters in an equation for the excess Gibbs energy of mixing was

described. The report of November 13 contained an example of the comparison between observed and calculated properties of the water-methanol system. For the past month, they have been gathering and selecting data for the five simple alcohols up through 1-butanol and entering these on cards for the computer calculations. Some preliminary runs have also been made.

They have also run an extensive series of tests on the computer calculation using sets of "synthetic data". These have served to check the programs for errors, as well as to determine the accuracy of the calculations of the parameters and thermodynamic properties. These tests have also given some basis to judge the effect of various kinds of data errors on the calculated values. These have shown, for example, the importance of having at least some calorimetric data in order to obtain reliable values of all of the thermodynamic properties.

Finally, an additional computer program has been written to calculate a table of thermodynamic properties from the parameters obtained in the least squares calculation. An example of the output of this program is included in the December 8 report. Fifteen parameters are calculated.

**Selected Heats of Combustion and Heats of Formation of
Organic Compounds of Biological Interest**

Eugene S. Domalski

I. Introduction

Selected values have been chosen for the heats of combustion and formation at 298°K for 174 organic compounds which have been divided into the following classes: additional aliphatic amino acids, aromatic amino acids, steroids, aliphatic dicarboxylic acids, hydroxy aliphatic dicarboxylic acids, aromatic and phenylated acids, anhydrides, oligosaccharides, methyl esters of aliphatic and aromatic monobasic acids, dimethyl esters of aliphatic and aromatic dibasic acids, aliphatic and aromatic amides, organic sulfur compounds, and organic phosphorus compounds.

Summing the total number of organic compounds treated in the present and three preceding reports (NBS reports 9883, 9968, and 10070) gives 682 for a final total. This collection of data will be arranged appropriately for publication in the Handbook of Thermodynamic Properties of Biological Materials.

II. Data on the Heats of Combustion and Formation of Various Classes of Organic Compounds

Additional Aliphatic Amino Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K$ kcal mol ⁻¹	References
γ -aminobutyric acid	c	-545.5	-138.1	[1]
δ -aminovaleric acid	c	-701.5	-144.5	[1]
α -aminocaproic acid(*)	c	-855.6	-152.7	[1,49]
γ -aminocaproic acid	c	-853.9	-154.5	[1]
δ -aminocaproic acid	c	-854.6	-153.7	[1]
ϵ -aminocaproic acid	c	-855.6	-152.7	[1]
zeta-aminoenanthic acid	c	-1011.1	-159.6	[1]
ω -aminopelargonic acid	c	-1321.4	-174.1	[1]
hexamethylene-1,6-diamine- adipic acid adduct	c	-1711.2	-305.5	[1]
tetramethylene-1,4-diamine- sebacic acid adduct	c	-2023.5	-317.9	[1]

(*)Also known as norleucine.

Aromatic Amino Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K$ kcal mol ⁻¹	References
o-aminobenzoic acid	c	-801.7	-95.8	[2]
m-aminobenzoic acid	c	-799.3	-98.2	[2]
p-aminobenzoic acid	c	-798.7	-98.8	[2]

Steroids

Compounds	State	$\Delta H_c^\circ, 298^\circ K$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K$ kcal mol ⁻¹	References
5 α -androstande	c	-2805	-75	[3]
5 α -androstande-3 α -ol-17-one (androsterone)	c	-2650	-162	[3]
5 α -androstande-3 β -ol-17-one (epiandrosterone)	c	-2660	-152	[3]
5 α -androstande-3 one-17 β -ol	c	-2692	-120	[3]
5 α -androstande-3,17-dione	c	-2613	-130	[3]
Δ_4 -androstande-3-one-17 β -ol (testosterone)	c	-2649	-94	[3]
Δ_5 -androstande-3 β -ol-17-one (trans-dehydroandrosterone)	c	-2636	-107	[3]
Δ_4 -androstande-3,17-dione	c	-2572	-103	[3]
Δ_4 -pregnene-3,20-dione (progesterone)	c	-2868	-132	[3]
Δ_4 -pregnene-3,20-dione-21-ol (desoxycorticosterone or cortexone)	c	-2876	-124	[3]
Δ_4 -pregnene-3,11,20-trione- 17 α ,21-diol (cortisone)	c	-2676	-244	[3]
Δ_4 -pregnene-3,20-dione- 11 β ,17 α ,21-triol (cortisol)	c	-2744	-256	[3]
5 β -cholan-24-oic acid-3 α ,7 α ,12 α - triol (cholic acid)	c	-3404	-288	[16,17]
Δ_5 -cholestene-3 β -ol (cholesterol)	c	-3677	-134	[3,31,32]
cholesteryl methyl ether	c	-4117.1	-155.9	[48]

Aliphatic Dicarboxylic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K,$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K,$ kcal mol ⁻¹	References
oxalic acid	c	-58.7	-197.7	[6-13, 33]
oxalic acid dihydrate	c	-52.0	-341.0	[14, 15, 33]
malonic acid	c	-205.82	-212.96	[6, 8, 9, 11, 13, 18, 19]
succinic acid	c	-356.31	-224.84	[6-9, 11, 13, 18-29]
glutaric acid	c	-514.08	-229.44	[9, 11, 13, 30]
adipic acid	c	-668.3	-237.6	[9, 11]

Hydroxy Aliphatic Dicarboxylic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}_1$ kcal mol ⁻¹	References
D-tartaric acid	c	-274.7	-306.5	[6, 7, 8, 34, 35, 36]
DL-tartaric acid	c	-272.6	-308.6	[34-39]
meso-tartaric acid	c	-275.3	-305.9	[34, 35, 36]
DL-tartaric acid monohydrate	c	-277	-372	[37, 38, 39]
L-malic acid	c	-317.37	-263.78	[13]
DL-malic acid	c	-316.88	-264.27	[13]
α -ketoglutaric acid	c	-429.85	-245.35	[42]
DL-trihydroxyglutaric acid	c	-388	-356	[44]
citric acid (anhydrous)	c	-468.6	-369.0	[6-9, 13, 18]
citric acid (monohydrate)	c	-468.27	-437.61	[18, 43]
allomucic acid	c	-494	-412	[44]
mucic acid	c	-483	-423	[45]

Unsaturated Aliphatic Dicarboxylic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	References
citraconic acid	c	-478.16	-197.04	[18, 40, 42, 45, 46]
itaconic acid	c	-474.14	-201.03	[18, 40, 42, 45]
mesaconic acid	c	-478	-197	[18, 40]
hexa-2-ene-1,6-dioic acid	c	-629	-209	[45]
hexa-3-ene-1,6-dioic acid	c	-629	-209	[45]
cis-aconitic acid	c	-476.6	-292.7	[18, 42, 45]
trans-aconitic acid	c	-474.6	-294.6	[18, 42, 45]
tetraconic acid	c	-796	-204	[37, 38, 47]

Aliphatic Amides

Compound	State	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	References
formamide	liq	-135.8	-60.7	[75,76,81]
urea	c	-151.12	-79.56	[7,8,58,61-69]
urea nitrate	c	-130.0	-134.8	[70,71]
guanidine	c	-251.45	-13.39	[82]
guanylurea nitrate	c	-325.1	-102.1	[50]
diaminoguanidine nitrate	c	-329.7	-37.6	[51]
nitroaminoguanidine	c	-270.1	+5.3	[51]
acetamide	c	-282.9	-76.0	[60,74,75,76]
formylurea	c	-207	-118	[52,53]
oxamide	c	-201.7	-123.0	[54,77,78]
malonamide	c	-356.6	-130.5	[21,77,78]
oxamic acid	c	-130.2	-160.4	[52,77,78]
azadipic acid	c	-254.82	-69.91	[55]
hydrazodicarbamide	c	-273.86	-119.91	[55]
N,N-dimethylformamide	liq	-464.1	-57.2	[56]
ethylcarbamate (urethane)	c	-396.9	-124.4	[77,78]
hydantoic acid	c	-308	-179	[52]
propionamide	c	-439.6	-81.7	[74,75,76]
guanidine carbonate	c	-459.95	-232.10	[57,58]
diacetamide	c	-498	-117	[59]
succinamide	c	-510.6	-138.9	[54,77,78]
D-tartramide	c	-426.6	-222.9	[34,54]
meso-tartramide	c	-426.0	-223.5	[34]
n-butyramide	c	-596.1	-87.5	[75,76]

Aromatic Amides

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
benzamide	c	-849.04	-48.42	[72-76]
formanilide	c	-861.2	-36.2	[75, 76]
phthalamide	c	-921.3	-104.4	[77, 78]
acetanilide	c	-1009.5	-50.3	[74, 75, 76, 83]
phenacetin	c	-1283.5	-101.1	[79, 80]
benzanilide	c	-1576.1	-22.3	[74, 75, 76]

Aromatic and Phenylated Aliphatic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
benzoic acid	c	-771.27	-92.03	[6-8, 84-119]
salicylic acid	c	-722.64	-140.66	[6, 8, 87, 120-136]
o-phthalic acid	c	-770.44	-186.92	[6, 8, 18, 45, 87, 137-139]
m-phthalic acid	c	-765.44	-191.91	[87, 137, 139]
p-phthalic acid	c	-762.30	-195.05	[87, 137]
phenylacetic acid	c	-930.3	-95.4	[6, 67, 87, 88, 91, 140, 141]
L-mandelic acid	c	-886.9	-138.8	[67, 121, 142]
DL-mandelic acid	c	-887.2	-138.5	[67, 121, 142]
phenylglyoxylic acid	c	-842.1	-115.3	[143]
phenoxyacetic acid	c	-902.9	-122.8	[67, 121]
DL-phenylglyceric acid	c	-1009.5	-178.5	[144]

Anhydrides

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
acetic anhydride	liq	-431.65	-149.50	[79,83]
maleic anhydride	c	-332.10	-112.42	[13,18,37,38, 47,145]
succinic anhydride	c	-369.0	-143.8	[18,67,146]

Oligosaccharides

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
raffinose	c	-2025	-761	[8,164]
raffinose pentahydrate	c	-2006	-1122	[14,15]
melezitose	c	-1971	-815	[165]
diamylose	c	-2774	-850	[166,167]
stachyose	c	-2705	-987	[166]
α -tetamylose	c	-4075	-1360	[166,167]
β -hexamylose	c	-5394	-1853	[166,167]

Methyl Esters of Monobasic Aliphatic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
methyl formate	g	-241.0	-83.7	[147, 148]
methyl formate	liq	-234.1	-90.6	[149-152]
methyl acetate	liq	-380.7	-106.4	[153]
methyl valerate	liq	-851.31	-122.89	[154, 155]
methyl caproate	liq	-1007.46	-129.10	[154]
methyl enanthate	liq	-1163.40	-135.53	[154]
methyl caprylate	liq	-1320.22	-141.07	[154]
methyl pelargonate	liq	-1476.37	-147.29	[154]
methyl caprate	liq	-1632.96	-153.07	[154]
methyl undecylate	liq	-1789.42	-158.97	[154]
methyl laurate	liq	-1945.10	-165.66	[154]
methyl tridecylate	liq	-2101.56	-171.56	[154]
methyl myristate	liq	-2257.69	-177.80	[154]
methyl pentadecylate	liq	-2413.51	-184.34	[154]
methyl oleate	liq	-2842.4	-174.3	[156, 157, 158]
methyl elaidate	liq	-2840.8	-175.8	[156, 157, 158]

Methyl Esters of Monobasic Aromatic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
methyl benzoate	liq	-945.9	-79.8	[84]
methyl salicylate	liq	-898.6	-127.1	[159, 160]

Dimethyl Esters of Dibasic Aliphatic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
dimethyl oxalate	liq	-400.2	-181.0	[41,161]
dimethyl malonate	liq	-553.3	-190.2	[161,162,163]
dimethyl succinate	liq	-706.3	-199.6	[41,161]
dimethyl maleate	liq	-669.4	-168.2	[37,38,47]
dimethyl fumarate	liq	-663.3	-174.3	[37,38,41,47]
dimethyl glutarate	liq	-862.3	-205.9	[161]
dimethyl adipate	liq	-1018.7	-211.9	[161]

Dimethyl Esters of Dibasic Aromatic Acids

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
dimethyl o-phthalate	liq	-1120.1	-162.0	[41]
dimethyl m-phthalate	c	-1111.0	-171.1	[41]
dimethyl p-phthalate	c	-1111.8	-170.3	[41,67]

Organic Sulfur Compounds

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
methanethiol	liq	-363.48	-11.08	[169]
ethanethiol	liq	-519.39	-17.53	[171,172]
1-propanethiol	liq	-675.51	-23.78	[179]
1-butanethiol	liq	-831.97	-29.69	[184]
1-pentanethiol	liq	-988.30	-35.72	[170,171, 176,200,201]
1-hexanethiol	liq	-1144.55	-44.84	[188]
2-thiapropane	liq	-521.37	-15.55	[172]
2,3-dithiabutane	liq	-665.98	-14.82	[173,174]
1,2-ethanedithiol	liq	-667.97	-12.83	[175]
1,3-propanedithiol	liq	-824.34	-18.76	[175]
1,4-butanedithiol	liq	-980.42	-25.05	[175]
thiacyclopropane	liq	-481.02	+12.41	[170,202]
thiacyclobutane	liq	-637.03	+6.05	[170,176, 200,202]
thiacyclopentane	liq	-775.86	-17.48	[170,176, 180,200,202]
thiacyclohexane	liq	-930.33	-25.32	[170,187 200,202]
thiophene	liq	-675.74	+19.03	[170,174,181- 183,189,200]
2-methylthiophene	liq	-829.83	+10.75	[185]
3-methylthiophene	liq	-829.46	+10.38	[186]
benzenethiol	liq	-928.45	+15.32	[195]
benzyl mercaptan	liq	-1086.0	+10.5	[196,197]
phenyl methyl sulfide	liq	-1087.0	+11.5	[197,198]
diphenyl sulfide	c	-1653.2	+39.1	[197,199]
diphenyl disulfide	c	-1793.7	+35.7	[197,199]

Organic Sulfur Compounds
(continued)

Compound	State	$\Delta H_c^\circ, 298^\circ K_1$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K_1$ kcal mol ⁻¹	References
thiolacetic acid	liq	-416.22	-52.39	[170,189]
β -thiolactic acid	liq	-519.4	-111.6	[177,178]
β,β -dithiolactic acid	liq	-962.7	-230.9	[177,178]
thiourea	c	-353.43	-21.13	[52,189,190]
2-aminoethane-1-sulfonic acid (taurine)	c	-383.4	-187.7	[191]
thiohydantoin	c	-503.2	-59.5	[192]
thiohydantoic acid	c	-498.4	-132.6	[192]
4-methylthiazole	liq	-707.18	+16.31	[193]
4 cyanothiazole	c	-641.03	+52.64	[193]
tetramethylthiuram monosulfide	c	-1417.43	+11.60	[194]
tetramethylthiuram disulfide	c	-1559.64	+9.94	[194]

Organic Phosphorus Compounds

Compound	State	$\Delta H_{\text{c}}^{\circ}, 298^{\circ}\text{K}_1$ kcal mol ⁻¹	$\Delta H_{\text{f}}^{\circ}, 298^{\circ}\text{K}_1$ kcal mol ⁻¹	References
trimethylphosphine	liq	-763	-30	[203]
triethyl phosphate	liq	-982	-297	[204, 206]
tri-n-propyl phosphate	liq	-1452	-315	[205]
tri-n-butyl phosphate	liq	-1906 (-1921)	-348 (-333)	[205, 206]
triisobutyl phosphate	liq	-1908	-346	[206]
tri-n-butyl phosphine oxide	c	-2143	-110	[205]
n-butyl ester of di-n-butylphosphinic acid	liq	-2071	-182	[205]
triphenyl phosphate	c	-2229	-181	[206]

III. Selection of the Combustion Data

Additional Aliphatic Amino Acids

The combustion data taken from Strepikheev et al. [1] were corrected from ΔH_c° at 20°C to ΔH_c° at 25°C.

α -aminocaproic acid (norleucine) - Although essentially identical, the combustion data from Strepikheev et al. [1] are preferred to Skuratov [49]. This supersedes the data found on page 4 of NBS Report 9968.

Steroids

Although the microcalorimetric techniques used by Paoli et al. [3] allowed measurements to be performed on small amounts of sample, heats of combustion of around 2800 kcal mol⁻¹ have a precision of 6 to 7 kcal mol⁻¹.

5 α -androstan-3-one-17 β -ol - The heat of combustion reported by Paoli et al. [3] is 170 kcal mol⁻¹ less negative than the value we cite. The value we selected was obtained by an energy-structure correlation which appeared to be more consistent with the other combustion data on the steroids. Paoli et al. [3] also have reservations on the reliability of their experimental combustion value for this compound.

Δ_5 -cholestene-3 β -ol (cholesterol) - The selection was obtained by averaging the data of Paoli et al. [1] and Berthelot and Andre [31,32].

Aliphatic Dicarboxylic Acids

oxalic acid - The combustion data of Becker and Roth [33] on oxalic acid dihydrate were combined with their data on the heats of solution of anhydrous oxalic acid and oxalic acid dihydrate to obtain the selected value.

oxalic acid dihydrate - The combustion data of Becker and Roth [33] were preferred to that of Jorrisen and van de Stadt [14,15].

malonic acid - The combustion data of Wilhoit and Shaio [13] were used to make the selection.

succinic acid - The combustion data of Keith and Mackle [28], Pilcher and Sutton [27], Cass, Springall, and Quincey [26], Huffman [22], and Wilhoit and Shaio [13] were averaged to obtain the selected value. The data of any of the above authors agree with the selected value by less than $0.1 \text{ kcal mol}^{-1}$. The data of Verkade, Hartman, and Coops [11] and Skuratov et al. [25] agree by about $0.2 \text{ kcal mol}^{-1}$.

glutaric acid - The combustion data of Wilhoit and Shaio [13] were used to obtain the selection.

adipic acid - The combustion data of Verkade, Hartman, and Coops [11] were used to make the selection.

Hydroxy Aliphatic Dicarboxylic Acids

D-tartaric acid - The combustion data of Coops and Verkade [34] were chosen to make the selection.

DL-tartaric acid - The combustion data of Coops and Verkade [34] were chosen to make the selection.

meso-tartaric acid - The combustion data of Coops and Verkade [34] were chosen to make the selection.

DL-tartaric acid hydrate - The combustion data of Ossipov [37,38,39] were averaged to obtain the selection.

citric acid (anhydrous) - The combustion data of Wilhoit and Shaio [13] were used to make the selection.

citric acid monohydrate - The combustion data of Chappel and Hoare [43] were used to make the selection.

Unsaturated Aliphatic Dicarboxylic Acids

citraconic acid - The combustion data of Wilhoit and Lei [42] were used to make the selection.

itaconic acid - The combustion data of Wilhoit and Lei [42] were used to make the selection.

mesaconic acid - The later combustion data of Louguinine [18] were preferred to the earlier work [40].

cis- and trans-aconitic acids - The combustion data of Wilhoit and Lei [42] were used to make the selection.

Aliphatic Amides

formamide - The combustion data of Roth and Banse [81] and Stohmann and Schmidt [75,76] were used to obtain the selection.

urea - The combustion data of Huffman [58] and Mannson and Sunner [69] were averaged to make the selection.

urea nitrate - The combustion data of Medard and Thomas [70] were used to make the selection.

acetamide - The data of Calvet [60] on the heat of solution of acetamide in NaOH(aq) were used in preference to the combustion data of Berthelot and Fogh [74] and Stohmann and Schmidt [75,76].

oxamide - The combustion data of Tavernier and Lamouroux [54] were used to make the selection.

malonamide - The combustion data of Tavernier and Lamouroux [21] were used to make the selection.

oxamic acid - The combustion data of Matignon [52], Stohmann [77], and Stohmann and Hausmann [78] were averaged.

propionamide - The combustion data of Stohmann and Schmidt [75,76] were preferred to that of Berthelot and Fogh [74].

guanidine carbonate - The combustion data of Huffman [58] were preferred to that of Medard and Thomas [57].

succinamide - The combustion data of Tavernier and Lamouroux [54] were preferred to the earlier work.

D-tartramide - The combustion data of Coops and Verkade [34] were used in preference to that of Tavernier and Lamouroux [54].

Aromatic Amides

benzamide - Cole and Gilbert [72] corrected the combustion data of Anderson and Gilbert [73]. The corrected data were the basis of our selected value.

acetanilide - The data of Wadsö [83] on the heat of hydrolysis of acetanilide were used in preference to the early combustion data.

phenacetin - The combustion data of Roth [79] were preferred to that of Lemoult [80].

benzanilide - The combustion data of Stohmann and Schmidt [75,76] were preferred to that of Berthelot and Fogh [74].

Aromatic and Phenylated Aliphatic Acids

benzoic acid - The selected value was obtained by using $\Delta E_B = -26434 \text{ J g}^{-1}$, and applying the corrections for standard states and ΔnRT . The references give a chronological evolution of the use of benzoic acid as a standard in combustion bomb calorimetry.

salicylic acid - The combustion data of Verkade [134] were used to make the selection. The data of Beckers are in good agreement with the selection.

o-phthalic acid - The combustion data of Schwabe and Wagner [137] were used to make the selection. The data of Richardson and Parks [138] are in good agreement with the selection.

m-phthalic acid - The combustion data of Schwabe and Wagner [137] were used to obtain the selected value.

p-phthalic acid - The combustion data of Schwabe and Wagner [137] were used to obtain the selected value.

phenylacetic acid - The combustion data of von Amers and Roth [140] were used to obtain the selected value. The data of Wrede [91] are in good agreement with the selection.

L- and DL-mandelic acid - The combustion data of Zubareva et al. [142] were used in preference to the earlier work.

Anhydrides

acetic anhydride - The aminolysis data of Wadsö [83] were used in preference to the combustion data of Roth [79].

maleic anhydride - The combustion data of Wilhoit and Shaio [13] were used. The data of Parks, Mosley, and Peterson [145] are in good agreement with the selected value.

succinic anhydride - The combustion data of Verkade and Hartman [146] were used to obtain the selection.

Methyl Esters of Monobasic Aliphatic Acids

methyl formate (g) - The combustion data of Thomsen [147] was used in preference to that of Berthelot and Ogier [148].

methyl formate (liq) - The combustion data of Berthelot and Delepine [149,159] and Roth and Banse [151] were combined to obtain the selected value.

methyl valerate - The combustion data of Adriaanse, Dekker, and Coops [154] were used to obtain the selected value.

The combustion data of Adriaanse, Dekker, and Coops [154] were adjusted to the 1961 atomic weight scale because the data were based upon the moles of ester introduced into the bomb prior to an experiment.

Dimethyl Esters of Dibasic Aromatic Acids

dimethyl oxalate - The combustion data of Verkade, Coops, and Hartman [161] were preferred to those of Stohmann, Kleber, and Langbein [41].

dimethyl malonate - The combustion data of Verkade, Coops, and Hartman [161] were preferred to those of Guinchant [162,163].

dimethyl succinate - The combustion data of Verkade, Coops, and Hartman [161] were preferred to those of Stohmann, Kleber, and Langbein [41].

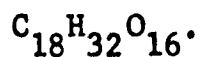
dimethyl fumarate - The combustion data of Stohmann, Kleber, and Langbein [41] and Ossipov [37,38,47] were averaged to obtain the selection.

Oligosaccharides

Generally speaking, the combustion data on the oligosaccharides are very poor because of insufficient characterization of the sample and because of the lack of precision and accuracy found in the early combustion measurements. The overall uncertainty in the combustion data is 2 to 4 percent.

raffinose - The bomb combustion data of Berthelot and Matignon [164] are preferred to the $KClO_3$ combustion data of Stohmann [8].

melezitose - Stohmann and Langbein [165] gave the formula, $C_{18}H_{34}O_7$, which is that for the monohydrate, but called the compound anhydrous, giving a melting point of $157^\circ C$. However, turanose, which is a hydrolysis product of melezitose, has a melting point of $157^\circ C$. Pigman and Goepf [168] cite a melezitose dihydrate with a melting point of $153-154^\circ C$. We have assumed the compound to be anhydrous in our calculations using the formula,



Organic Sulfur Compounds

We have used $H_2SO_4 \cdot 115H_2O(liq)$ as the final state for the sulfur in the heats of combustion of the organic sulfur compounds listed in this report, and have taken $\Delta H_f^\circ[H_2SO_4 \cdot 115H_2O(liq)] = -212.192 \text{ kcal mol}^{-1}$ at $25^\circ C$.

ethanethiol - The combustion data of McCullough, et al. [172] were preferred to the earlier work.

1-pentanethiol - As shown by Sunner [170] the combustion data at Lund and USBM are in good agreement, and difference only by $0.29 \text{ kcal mol}^{-1}$. We have chosen the value based on USBM data because it was in better agreement with the energy term for the CH_2 increment.

2,3-dithiabutane - The combustion data of Hubbard, et al. [173] were preferred to those of Franklin and Lumpkin [174].

thiacyclobutane - Sunner [170] has shown that the combustion data at Lund and USBM differ by only $0.24 \text{ kcal mol}^{-1}$. We have used the USBM data for our selection.

thiacyclopentane - Sunner [170] has shown that the combustion data at Lund and USBM differ by only $0.10 \text{ kcal mol}^{-1}$. We have used the USBM data for our selection.

thiacyclohexane - Sunner [170] has shown that the combustion data at Lund and USBM differ by only $0.05 \text{ kcal mol}^{-1}$. We have used the USBM data for our selection.

thiophene - The difference between the combustion data at Lund and those at USBM is $+0.35 \text{ kcal mol}^{-1}$. We have used the USBM data for our selected value.

thiourea - The combustion data of Sunner [189] were preferred to any earlier data.

Organic Phosphorus Compounds

The combustion data on organic phosphorus compounds is, in general, very poor. None of the measurements were made in a rotating-bomb calorimeter which would insure homogeneity of the phosphoric acid solution formed during the combustion. Appropriate data to provide the information needed for the reduction of the bomb process to standard conditions are not available. Most of the combustion data are uncertain from 0.25 to 0.5 percent. We have adjusted the combustion data so that $\text{H}_3\text{PO}_4(\text{c})$ appears as the final state of phosphorus, and have used $\Delta H_f^\circ[\text{H}_3\text{PO}_4(\text{c})] = -305.7$ kcal mol⁻¹.

triethyl phosphate - The combustion data of Bedford and Mortimer [204] were preferred to those of Nikolaev, Afanss'ev, and Starostin [206].

IV. References

- [1] Strepikheev, A. A., Skuratov, S. M., Shtekher, S. M., Muromova, R. S., Brykina, E. P., and Kachinskaya, O. N., Doklady Akad. Nauk SSSR 102, 543-545 (1955).
- [2] Lebedeva, N. D., Ryadnenko, B. L., and Gutner, N. M., First Int. Conf. on Calorimetry and Thermodynamics, Warsaw, Aug. 31 - Sept. 4, 1969, 8 pages.
- [3] Paoli, D., Garrigues, J.-C., and Patin, H., Compt. rend. C268, 780-783 (1969).
- [4] Berthelot, M., Ann. chim. et phys. [7] 20, 145-149 (1900).
- [5] Berthelot, M., Compt. rend. 129, 320-326 (1899).
- [6] von Rechenberg, C., J. prakt. Chem. [2] 22, 1-45 (1880).
- [7] Stohmann, F., von Rechenberg, C., Wilsing, H., and Rodatz, P., Landw. Jahrb. 13, 549-581 (1884).
- [8] Stohmann, F., J. prakt. Chem. [2] 31, 273-306 (1885).
- [9] Stohmann, F., Kleber, C., and Langbein, H., J. prakt. Chem. [2] 40, 202-229 (1889).
- [10] Jahn, H., Ann. Physik 37, 408-443 (1889).
- [11] Verkade, P. E., Hartman, H., and Coops, J., Rec. trav. chim. 45, 373-393 (1926).
- [12] Pässler, W., and König, W., Z. angew. Chem. 44, 288-291 (1931).
- [13] Wilhoit, R. C., and Shiao, D., J. Chem. Eng. Data 9, 595-599 (1964).
- [14] Jorrisen, W. J., and van de Stadt, E., J. prakt. Chem. [2] 51, 102-106 (1895).
- [15] Jorrisen, W. J., and van de Stadt, E., Maandb. Natuurw., Amsterdam, 1894, 6-10.
- [16] Berthelot, M., Ann. chim. et phys. [7] 20, 145-149 (1900).

- [17] Berthelot, M., Compt. rend. 129, 320-326 (1899).
- [18] Louguinine, W., Ann. chim. et phys. [6] 23, 179-231 (1891).
- [19] Louguinine, W., Compt. rend. 107, 597-600 (1888).
- [20] Beckers, M., Bull. soc. chim. Belges, 40, 571-610 (1931).
- [21] Tavernier, P., and Lamouroux, M., Mem. poudres, 37, 197-205 (1955).
- [22] Huffman, H. M., J. Am. Chem. Soc. 60, 1171-1177 (1938).
- [23] Roth, W. A., Z. Electrochem. 43, 355-356 (1937).
- [24] Breitenbach, J. W. and Derkosch, J., Monatsh. 82, 177-179 (1951).
- [25] Skuratov, S. M., Strepikheev, A. A., Kachinskaya, O. N., Shtekher, S. M., and Brykina, E. P., Uchenye Zapiski Moskov. Gosudarst. Univ. im. M. V. Lomonosova, No. 164, 73-85 (1953).
- [26] Cass, R. C., Springall, H. D., and Quincey, P. G., J. Chem. Soc. 1955, 1188-1190.
- [27] Filcher, G., and Sutton, L. E., Phil. Trans. Roy. Soc. (London) Ser. A, 248, 23-44 (1955).
- [28] Keith, W. A., and Mackle, H., Trans. Faraday Soc. 54, 353-366 (1958).
- [29] Miroshnichenko, E. A., Leiko, V. P., and Lebedev, Yu. A., Zhur. Fiz. Khim. 38, 1054-1055 (1964).
- [30] Stohmann, F., and Kleber, C., J. prakt. Chem. [2] 45, 475-499 (1892).
- [31] Berthelot, M., and Andre, G., Ann. chim. et phys. [7] 17, 433-451 (1899).
- [32] Berthelot, M., and Andre, G., Compt. rend. 128, 959-971 (1899).
- [33] Becker, G., and Roth, W. A., Z. Electrochem. 40, 836-843 (1934).
- [34] Coops, J., and Verkade, P. E., Rec. trav. chim. [4] 44, 983-1011 (1925).
- [35] Blanck, H. C., and Wolf, K. L., Z. physik. Chem. 32B, 139-144 (1936).

- [36] Dunken, H., and Wolf, K. L., *Z. physik. Chem.* 38B, 441-450 (1938).
- [37] Ossipov, I., *Ann. chim. et phys.* [6] 20, 371-403 (1890).
- [38] Ossipov, I., *Compt. rend.* 109, 475-476 (1889).
- [39] Ossipov, I., *Compt. rend.* 108, 1105-1108 (1889).
- [40] Louguinine, W., *Compt. rend.* 106, 1289-1291 (1888).
- [41] Stohmann, F., Kleber, C., and Langbein, H., *J. prakt. Chem.* [2] 40, 341-364 (1889).
- [42] Wilhoit, R. C., and Lei, I., *J. Chem. Eng. Data* 10, 166-168 (1965).
- [43] Chappel, F. P., and Hoare, F. E., *Trans. Faraday Soc.* 54, 367-371 (1958).
- [44] Fogh, J., *Compt. rend.* 114, 920-923 (1892).
- [45] Stohmann, F., *Z. physik. Chem.* 10, 410-424 (1892).
- [46] Stohmann, F., unpublished data quoted in Liebermann, C., *Ber.* 25, 90-95 (1892).
- [47] Ossipov, I., *Compt. rend.* 109, 311-312 (1889).
- [48] Jaffe, I., and Prosen, E. J., in Shoppee, C. W., and Williams, D. F., *J. Chem. Soc.* 1956, 2488-2491.
- [49] Skuratov, S. M., Doctorial Thesis, Moscow State Univ., 1953. cited in Ponomarev, V. V., *Zhur. Fiz. Khim.* 36, 1472-1476 (1962).
- [50] Söll, J., and Stutzer, A., *Ber.* 42, 4532-4541 (1909).
- [51] McEwan, W. S., and Riggs, M. W., *J. Am. Chem. Soc.* 73, 4725-4727 (1951).
- [52] Matignon, C., *Ann. chim. et phys.* [6] 28, 70-125 (1893).
- [53] Matignon, C., *Compt. rend.* 112, 1367-1369 (1891).
- [54] Tavernier, P., and Lamouroux, M., *Mem. poudres* 39, 335-356 (1957).

- [55] Williams, M. M., McEwan, W. S., and King, R. A., J. Phys. Chem. 61, 261-267 (1957).
- [56] Medard, L., and Thomas, M., Mem. poudres 39, 195-208 (1957).
- [57] Medard, L., and Thomas, M., Mem. poudres 37, 129 (1955).
- [58] Huffman, H. M., J. Am. Chem. Soc. 62, 1009-1011 (1940).
- [59] Parts, A., Z. physik. Chem. 131, 405-408 (1928).
- [60] Calvet, E., J. chim. phys. 30, 140-166 (1933).
- [61] Emery, A. G., and Benedict, F. G., Am. J. Physiol. 28, 301-307 (1911).
- [62] Berthelot, M., and Petit, P., Ann. chim. et phys. [6] 20, 13-20 (1890).
- [63] Berthelot, M., and Petit, P., Compt. rend. 109, 759-764 (1889).
- [64] Krummacher, O., Z. Biol. 46, 302-321 (1905).
- [65] Ruehrwein, R. A., and Huffman, H. M., J. Am. Chem. Soc. 68, 1759-1761 (1946).
- [66] Stohmann, F., and Langbein, H., J. prakt. Chem. [2] 44, 336-399 (1891).
- [67] Stohmann, F., Z. physik. Chem. 6, 334-357 (1890).
- [68] Rubner, M., Z. Biol. 21, 251-334 (1885).
- [69] Mannson, M., and Sunner, S., Acta Chem. Scand 17, 723-727 (1923).
- [70] Medard, L., and Thomas, M., Mem. poudres 31, 173-196 (1949).
- [71] Schmidt, A., Z. ges. Schies. u. Sprengstoffw. 29, 259-266 (1934).
- [72] Cole, L. G., and Gilbert, E. C., J. Am. Chem. Soc. 73, 5423-5427 (1951).
- [73] Anderson, C. M., and Gilbert, E. C., J. Am. Chem. Soc. 64, 2369-2372 (1942).

- [74] Berthelot, M., and Fogh, J., Ann. chim. et phys. [6] 22, 18-24 (1891).
- [75] Stohmann, F., and Schmidt, R., Ber. Verhandl. K. Sachs. Ges. Wiss. Math.-Phys. Kl. 47, 1-36 (1895).
- [76] Stohmann, F., and Schmidt, R., J. prakt. Chem. [2] 52, 59-71 (1895).
- [77] Stohmann, F., Ber. Verhandl. K. Sachs. Ges. Wiss. Math.-Phys. Kl. 49, 1-74 (1897).
- [78] Stohmann, F., and Haussmann, E., J. prakt. Chem. [2] 55, 263-284 (1897).
- [79] Roth, W. A., Rec. trav. chim. 45, 248-256 (1926).
- [80] Lemoult, P., Compt. rend. 143, 772-775 (1906).
- [81] Roth, W. A., and Bause, H., unpublished data quoted in Landolt-Börnstein Phys. Chem. Tabellen, 5th Edition, Ergb. III, 2906 (Verlag J. Springer, Berlin, 1936).
- [82] Kirpichev, E. P., Titov, L. V., Rubstov, Yu. I., and Gavrilova, L. A., Zhur. Fiz. Khim. 42, 512-513 (1968).
- [83] Wadsö, I., Acta Chem. Scand. 16, 471-478 (1962).
- [84] Stohmann, F., Rodatz, P., and Herzberg, W., J. prakt. Chem. [2] 36, 1-16 (1887).
- [85] Berthelot, M., and Louguinine, W., Ann. chim. et phys. [6] 13, 321-339 (1888).
- [86] Berthelot, M., and Recoura, A., Ann. chim. et phys. [6] 13, 304-320 (1888).
- [87] Stohmann, F., Kleber, C., and Langbein, H., J. prakt. Chem. [2] 40, 128-157 (1889).
- [88] Fischer, E., and Wrede, F., Sitz. ber. preuss., Akad. Wiss. 687-715 (1904).
- [89] Fischer, E., and Wrede, F., Sitz. ber. preuss., Akad. Wiss. 124-146 (1908).
- [90] Fischer, E., and Wrede, F., Z. physik. Chem. 69, 218-235 (1909).

- [91] Wrede, F., Z. physik. Chem. 75, 81-94 (1910).
- [92] Roth, W. A., Ann. 373, 249-266 (1910).
- [93] Swietoslowski, W., and Popov, M., Zhur. Russ. Fiz. Khim. Obshchestva, Chast Khim. 46, 935-975 (1914).
- [94] Swietoslowski, W., and Pakovich, I., Zhur. Russ. Fiz. Khim. Obshchestva, Chast Khim. 46, 1284-1293 (1914).
- [95] Swietoslowski, W., Popov, M., and Pakovich, I., Zhur. Russ. Fiz. Khim. Obshchestva, Chast Khim. 46, 1293-1301 (1914).
- [96] Swietoslowski, W., Zhur. Russ. Fiz. Khim. Obshchestva Chast Khim. 46, 1302-1310 (1914).
- [97] Dickinson, H. C., Bull. Bur. Standards 11, 189-257 (1915).
- [98] Swietoslowski, W., J. Am. Chem. Soc. 39, 2595-2600 (1917).
- [99] Penning, F., Z. physik. Chem. 97, 467-477 (1921).
- [100] Swietoslowski, W., Roczniki Chem. 1, 59-103 (1921).
- [101] Swietoslowski, W., and Starczewska, H., Bull. soc. chim. France [4] 31, 654-667 (1922).
- [102] Roth, W. A., Doepke, O., and Banse, H., Z. physik. Chem. 133, 431-442 (1928).
- [103] Jaeger, W., and von Steinwehr, H., Z. physik. Chem. 135, 305-346 (1928).
- [104] Landrieu, P., Baylocq, F., and Johnson, J. R., Bull. soc. chim. France [4] 45, 36-49 (1929).
- [105] Jessup, R. S., and Green, C. B., J. Research NBS 13, 469-495 (1934).
- [106] Jessup, R. S., J. Research NBS 29, 247-270 (1942).
- [107] Prosen, E. J., and Rossini, F. D., J. Research NBS 33, 439-446 (1944).
- [108] Jessup, R. S., J. Research NBS 36, 421-423 (1946).
- [109] Magnus, A., and Becker, F., Erdöl u. Kohle 4, 115-118 (1951).

- [110] Challoner, A. R., Gundry, H. A., and Meetham, A. R., *Phil. Trans. Roy. Soc. (London)* 247A, 553-582 (1955).
- [111] Magnus, A., *Z. physik. Chem. [N.F.]* 9, 141-161 (1956).
- [112] Coops, J., Adriaanse, N., and Van Nes, K., *Rec. trav. chim.* 75, 237-253 (1956).
- [113] Gundry, H. A., and Meetham, A. R., *Trans. Faraday Soc.* 54, 664-670 (1958).
- [114] Meetham, A. R., and Nicholls, J. B., *Proc. Roy. Soc. (London)* 256A, 384-399 (1960).
- [115] Oleinik, B. N., and Uskov, V. S., *Zhur. Fiz. Khim.* 38, 2162-2164 (1964).
- [116] Peters, H., and Toppe, E., *Monatsber. Deut. Akad. Wiss. Berlin*, 9, 828-837 (1967).
- [117] Churney, K. L., and Armstrong, G. T., *J. Research NBS* 72A, 453-465 (1968).
- [118] Mosselman, C., and Dekker, H., *Rec. trav. chim.* 88, 161-176 (1969).
- [119] Gundry, H. A., Harrop, D., Head, A. J., and Lewis, G. B., *J. Chem. Thermodynamics* 1, 321-332 (1969).
- [120] Delepine, M., and Rivals, P., *Compt. rend.* 129, 520-523 (1899).
- [121] Stohmann, F., and Langbein, H., *Ber. Verhandl. K. Sachs. Ges. Wiss., Math. Phys. Kl.* 46, 226-251 (1894).
- [122] Roth, W. A., and Lasse, R., *Z. Electrochem.* 30, 607-609 (1924).
- [123] Keffler, L. J. P., and Guthrie, F. C., *J. Phys. Chem.* 31, 58-68 (1927).
- [124] Keffler, L. J. P., *J. Phys. Chem.* 33, 37-51 (1929).
- [125] Keffler, L. J. P., *Rec. trav. chim.* 49, 428-440 (1930).
- [126] Keffler, L. J. P., *J. chim. phys.* 28, 457-469 (1931).
- [127] Berner, E., *J. Chem. Soc.* 127, 2747-2750 (1925).

- [128] Berner, E., J. Chem. Soc. 1927, 338-341.
- [129] Milone, M., and Rossignoli, P., Gazz. chim. et al. 62, 644-655 (1932).
- [130] Cohen, E., Verkade, P. E., Miyake, S., Coops, J., and van der Hoeve, J. A., Verslag Gewone Vergader. Afdel. Natuurk. Ned. Akad. Wetenschap. 35, 48-53 (1926).
- [131] Cohen, E., Verkade, P. E., Miyake, S., Coops, J. and van der Hoeve, J. A., Z. physik. Chem. 126, 290-296 (1927).
- [132] Verkade, P. E., and Coops, J. Rec. trav. chim. 43, 561-581 (1924).
- [133] Verkade, P. E., and Coops, J., J. Chem. Soc. 1926, 1437-1443.
- [134] Verkade, P. E., and Coops, J. Rec. trav. chim. 47, 709-714 (1928).
- [135] Beckers, M., Bull. soc. chim. Belges, 40, 518-570 (1931).
- [136] Verkade, P. E., J. chim. phys. 29, 297-301 (1932).
- [137] Schwabe, K., and Wagner, W., Z. Electrochem. 65, 812-814 (1961).
- [138] Richardson, J. W., and Parks, G. S., J. Am. Chem. Soc. 61, 3543-3546 (1939).
- [139] Verkade, P. E., and Hartman, H., unpublished data quoted in Verkade, P. E., Verslag Gewone Vergader. Afdel. Natuurk. Koninkl. Ned. Akad. Wetenschap 35, 492 (1926).
- [140] von Auwers, K., and Roth, W. A., Ann. 373, 239-248 (1910).
- [141] Stohmann, F., and Schmidt, R., J. prakt. Chem. [2] 53, 345-369 (1896).
- [142] Zubareva, N. D., Oberemok-Yakubova, A. P., Petrov, Yu. I., Klabunovskii, and Balandin, A. A., Izvest. Akad. Nauk SSSR, Ser. Khim. 1963, 2207.
- [143] Neuberg, C., and Hofmann, E., Biochem. Z. 252, 440-450 (1932).
- [144] Berner, E., Tidskr. Kem. 16, 97, 118 (1919).
- [145] Parks, G. S., Mosley, J. R., and Peterson, P. V., J. Chem. Phys. 18, 152-153 (1950).
- [146] Verkade, P. E., and Hartman, H., Rec. trav. chim 52, 945-968 (1933).

- [147] Thomsen, J., Thermochemische Untersuchungen, vol. IV, 200 (1886).
- [148] Berthelot, M., and Ogier, J., Ann. chim. et phys. [5] 23, 201-209 (1881).
- [149] Berthelot, M., and Delepine, M., Ann. chim. et phys. [7] 21, 289-296 (1900).
- [150] Berthelot, M., and Delepine, M., Compt. rend. 130, 1045-1049 (1900).
- [151] Roth, W. A., and Banse, H., unpublished data quoted in Landolt-Börnstein Phys. Chem. Tabellen, 5th Edition, Ergb. III, 1634 (Verlag J. Springer, Berlin, 1936).
- [152] Favre, P. A., and Silbermann, J. T., Ann. chim. et phys. [3] 34, 357-450 (1852).
- [153] Roth, W. A., and Müller, F., unpublished data quoted in Landolt-Börnstein Phys. Chem. Tabellen, 5th Edition, Ergb. I, 876 (Verlag J. Springer, Berlin, 1927).
- [154] Adriaanse, N., Dekker, H., and Coops, J., Rec. trav. chim. 84, 393-407 (1965).
- [155] Hancock, C. K., Watsen, G. M., Gilby, R. F., J. Phys. Chem. 58, 127-129 (1954).
- [156] Keffler, L. J. P., J. Phys. Chem. 34, 1319-1325 (1930).
- [157] Keffler, and McLean, J. H., J. Soc. Chem. Ind. (London) 54, 178T-185T (1935).
- [158] Keffler, L. J. P., J. Phys. Chem. 41, 715-721 (1937).
- [159] Stohmann, F., Rodatz, P., and Herzberg, W., J. prakt. Chem. [2] 36, 353-370 (1887).
- [160] Sinke, G. C., unpublished results, Dow Chem. Co. quoted in "The Chemical Thermodynamics of Organic Compounds", Stull, D. R., Westrum, E. F., Jr., and Sinke, G. C., (John Wiley & Sons, Inc., New York, 1969), page 698.
- [161] Verkade, P. E., Coops, J., and Hartman, H., Rec. trav. chim. 45, 585-606 (1926).

- [162] Guinchant, J., Ann. chim. (Paris) [9] 10, 30-84 (1918).
- [163] Guinchant, J., Compt. rend. 121, 354-357 (1895).
- [164] Berthelot, M., and Matignon, C., Ann. chim. et phys. [6] 21, 409-416 (1890).
- [165] Stohmann, F., and Langbein, H., J. prakt. Chem. [2] 45, 305-356 (1892).
- [166] Karrar, P., and Floroni, W., Ber. 55B, 2854-2863 (1922).
- [167] Schläpfer, P., unpublished data in Karrar, P., Nägeli, C., Hurwitz, O., and Wälti, A., Helv. chim. Acta 4, 678-699 (1921).
- [168] Pigman, W. W., and Goepp, R. M., Jr., "Chemistry of the Carbohydrates" (Academic Press Inc., Publishers, New York, 1948).
- [169] Good, W. D., Lacina, J. L., and McCullough, J. P., J. Phys. Chem. 65, 2229-2231 (1961).
- [170] Sunner, S., Acta Chem. Scand. 17, 728-730 (1963).
- [171] Berthelot, M., Ann. chim. et phys. [7] 22, 322-326 (1901).
- [172] McCullough, J. P., Hubbard, W. N., Frow, F. R., Hossenlopp, I. A., and Waddington, G., J. Am. Chem. Soc. 79, 561-566 (1957).
- [173] Hubbard, W. N., Douslin, D. R., McCullough, J. P., Scott, D. W., Todd, S. S., Messerly, J. F., Hossenlopp, I. A., George, A., and Waddington, G., J. Am. Chem. Soc. 80, 3547-3554 (1958).
- [174] Franklin, J. L., and Lumpkin, H. E., J. Am. Chem. Soc. 74, 1023-1026 (1952).
- [175] Mannson, M., and Sunner, S., Acta Chem. Scand 16, 1863-1869 (1962).
- [176] Hubbard, W. N., Katz, C., and Waddington, G., J. Phys. Chem. 58, 142-152 (1954).
- [177] Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. 57, 41-46 (1935).
- [178] Borsook, H., Ellis, E. L., and Huffman, H. M., J. Biol. Chem. 117, 281-308 (1937).

- [179] Hubbard, W. N., and Waddington, G., *Rec. trav. chim.* 73, 910-923 (1954).
- [180] Davies, J. V., and Sunner, S., *Acta Chem. Scand* 16, 1870-1875 (1962).
- [181] Waddington, G., Knowlton, J. W., Scott, D. W., Oliver, G. D., Todd, S. S., Hubbard, W. N., Smith, J. C., and Huffman, H. M., *J. Am. Chem. Soc.* 71, 797-808 (1949).
- [182] Hubbard, W. N., Scott, D. W., Frow, F. R., and Waddington, G. *J. Am. Chem. Soc.*, 77, 5855-5857 (1955).
- [183] Moore, G. E., Renquist, M. L., and Parks, G. S., *J. Am. Chem. Soc.* 62, 1505-1507 (1940).
- [184] Hubbard, W. N., Good, W. D., and Waddington, G., *J. Phys. Chem.* 62, 614-617 (1958).
- [185] Pennington, R. E., Finke, H. L., and Hubbard, W. N., *J. Am. Chem. Soc.* 78, 2055-2060 (1956).
- [186] McCullough, J. P., Sunner, S., Finke, H. L., Hubbard, W. N., Gross, M. E., Pennington, R. E., Messerly, J. F., Good, W. D., and Waddington, G., *J. Am. Chem. Soc.* 75, 5075-5081 (1953).
- [187] McCullough, J. P., Finke, H. L., Hubbard, W. N., Good, W. D., Pennington, R. E., Messerly, J. F., and Waddington, G., *J. Am. Chem. Soc.* 76, 2661-2669 (1954).
- [188] Good, W. D., and DePrater, B. L., *J. Phys. Chem.* 70, 3606-3609 (1966).
- [189] Sunner, S., *Acta Chem. Scand.* 9, 847-854 (1955).
- [190] Becker, G., and Roth, W. A., *Z. physik. Chem.* A169, 287-296 (1934).
- [191] Berthelot, M., *Ann. chim. et phys.* [6] 28, 126-139 (1893).
- [192] Matignon, C., *Ann. chim. et phys.* [6] 28, 289-394 (1893).
- [193] Månsson, M., and Sunner, S., *Acta Chem. Scand.* 20, 845-848 (1966).
- [194] Good, W. D., Lacina, J. L., and McCullough, J. P., *J. Phys. Chem.* 65, 860-862 (1961).
- [195] Scott, D. W., McCullough, J. P., Hubbard, W. N., Messerly, J. F., Hossenlopp, I. A., Frow, F. R., and Waddington, G., *J. Am. Chem. Soc.*, 78, 5463-5468 (1956).

- [196] Mackle, H., and McClean, R. T. B., Trans. Faraday Soc. 58, 895-899 (1962).
- [197] Mackle, H., Queens' Univ. of Belfast, private communication. Oct. 30, 1964.
- [198] Mackle, H., and Mayrick, R. G., Trans. Faraday Soc. 58, 33-39 (1962).
- [199] Mackle, H., and Mayrick, R. G., Trans. Faraday Soc. 58, 238-243 (1962).
- [200] McCullough, J. P., Bur. of Mines, private communication in reference [170].
- [201] Sunner, S., Acta Chem. Scand. 9, 837-846 (1955).
- [202] Sunner, S., thesis, University of Lund, Sweden, 1949.
- [203] Long, L. H., and Sackman, J. F., Trans. Faraday Soc. 53, 1606-1611 (1957).
- [204] Bedford, A. F., and Mortimer, C. T., J. Chem. Soc. 1960, 1622-1625.
- [205] Starostin, A. D., Nikolaev, A. V., and Afanas'ev, Yu. A., Izvest. Akad. Nauk SSSR, Ser. Khim.; No. 8, 1303-1307 (1966).
- [206] Nikolaev, A. V., Afanas'ev, Yu. A., and Starostin, A. D., Doklady Akad Nauk SSSR 168, 351-353 (1966).

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