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NATIONAL BUREAU OF STANDARDS REPORT

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

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Progress Report for the Period 1 January to 30 June 1969
to
National Aeronautics and Space Administration



U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

NATIONAL BUREAU OF STANDARDS

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NATIONAL BUREAU OF STANDARDS REPORT

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

George T. Armstrong and Eugene S. Domalski

Progress Report for the Period 1 January to 30 June 1969
to

National Aeronautics and Space Administration

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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 sixteenth 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

George T. Armstrong

During this reporting interval further progress was made on the selection of heats of combustion of organic substances relevant to the program. This work was done largely by Dr. E. S. Domalski and his results for 115 organic compounds are presented as a chapter of this progress report, beginning on page 2.

During this interval arrangements were made to have much of the tabulated results of this work published by Academic Press, Inc. A manuscript deadline of July 1970 was accepted.

A portion of the funds of this contract are being used to obtain evaluations of thermodynamic properties of aqueous solutions of biologically important compounds from the Texas A and M Thermodynamics Research Center. Dr. R. A. Wilhoit is the scientist in charge of their contributions. This work was initiated in May 1969. The thermodynamics Research Center has submitted two monthly progress reports. The first reports consist of bibliographies on activity coefficients, partial molal enthalpies, partial molal heat capacities, and osmotic coefficients of the simpler organic acids and alcohols.

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

Eugene S. Domalski

I. Introduction

We report here selected values for the heats of combustion and formation at 298°K for the following classes of organic compounds: aliphatic hydrocarbons, alicyclic hydrocarbons, aromatic hydrocarbons, aliphatic alcohols, phenols, aliphatic di- and polyols, aldehydes, ketones, n-aliphatic acids, hydroxy aliphatic acids, and unsaturated aliphatic acids. The total number of compounds for which selected values have been made in this report is 115. Adding to this total, the compounds similarly treated in NBS Report 9883 (73 organic compounds), and NBS Report 9968 (321 organic compounds), we obtain 509 for a final total to date. A final portion of about 100 compounds will be processed for the next report.

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

Aliphatic Hydrocarbons

Compound	State	ΔH_c° 298°K kcal mol ⁻¹	ΔH_f° 298°K kcal mol ⁻¹	Reference
methane	g	-212.80	-17.88	[1,2,3,32,237,240,243]
ethane	g	-372.82	-20.23	[1,4,32,245]
propane	g	-530.60	-24.81	[1,4,32,245]
n-butane	g	-687.64	-30.14	[1,4]
n-pentane	g	-845.16	-34.99	[1,4,143]
n-pentane	liq	-838.69	-41.46	[1,5,246,248]
ethylene	g	-337.23	+12.50	[1,6,7,32,237,242,244,245,252]
acetylene	g	-310.62	+54.20	[1,8,32,33,244,245,252]

Alicyclic Hydrocarbons

Compound	State	ΔH_c° 298°K kcal mol ⁻¹	ΔH_f° 298°K kcal mol ⁻¹	Reference
cyclopropane	g	-499.85	+12.75	[1,9,244,245,253]
cyclobutane	liq	-650.22	+0.76	[1,10,11]
cyclopentane	liq	-786.55	-25.28	[1,11,12,13,17,254]
cyclohexane	liq	-936.87	-37.33	[1,10,12-20]
cycloheptane	liq	-1099.09	-37.47	[1,10,12,16,17]
cyclooctane	liq	-1258.58	-40.35	[1,10,12,21,22]

Aromatic Hydrocarbons

Compound	State	ΔH_c° 298°K kcal mol ⁻¹	ΔH_f° 298°K kcal mol ⁻¹	Reference
benzene	g	-789.06	+19.81	[1,23-37]
benzene	liq	-780.96	+11.71	[1,18,20,38-47]
naphthalene	g	-1249.4	+35.6	[48-58]
naphthalene	c	-1231.8	+18.0	[18,42,59-87]
anthracene	g	-1714.7	+53.7	[48,55,57,88-92]
anthracene	c	-1687.3	+29.0	[38,59,60,65,77, 78,80,83,86,87,93-100]
phenanthrene	g	-1706.7	+48.4	[48,55,90]
phenanthrene	c	-1685.6	+27.3	[38,65,80,83,87, 94-97,99,100]
pyrene	c	-1873.83	+27.44	[97,101]
triphenylene	c	-2136.53	+33.72	[99,101]
chrysene	c	-2137.8	+35.0	[99,102]
1,2-benzanthracene	c	-2144.0	+41.2	[99]
3,4-benzphenanthrene	c	-2147.3	+44.5	[99]
tetracene	c	-2141.1	+38.3	[99]
perylene	c	-2334.60	+43.69	[101,103]
fluoranthrene	c	-1892.14	+45.75	[101,104]

Aliphatic Alcohols

Compound	State	ΔH_C° , 298°K kcal mol ⁻¹	ΔH_F° , 298°K kcal mol ⁻¹	Reference
methanol	g	-182.72	-47.96	[32,105,112,237,238,239]
methanol	liq	-173.64	-57.04	[42,106-111]
ethanol	g	-336.86	-56.19	[32,105,237,239,240,241]
ethanol	liq	-326.68	-66.37	[42,109,111,113-117]
1-propanol	liq	-482.75	-72.66	[17,42,111,118-120]
2-propanol	liq	-479.44	-75.97	[17,111,118-120,126,127]
1-butanol	liq	-639.53	-78.25	[17,42,111,120-124,247]
2-butanol	liq	-635.90	-81.88	[111,121]
2-methyl-1-propanol	liq	-637.93	-79.85	[17,42,111,118,120,121]
2-methyl-2-propanol	liq	-631.92	-85.86	[17,120,121,128,129]
1-pentanol	liq	-795.25	-84.90	[17,111,118,120,123,125]
1-hexanol	liq	-951.70	-90.81	[111,123]

Phenols

Compound	State	ΔH_C° , 298°K kcal mol ⁻¹	ΔH_F° , 298°K kcal mol ⁻¹	Reference
phenol	c	-729.80	-39.45	[59,60,63,65,102,130-138]
pyrocatechol	c	-683.0	-86.3	[60,102,137]
resorcinol	c	-681.30	-87.95	[60,102,139]
hydroquinone	c	-681.78	-87.47	[63,102,134-137, 140-142,144,145]
o-cresol	c	-882.72	-48.90	[130-132,146]
m-cresol	c	-885.25	-46.37	[130-132,138,146,147]
p-cresol	c	-883.99	-47.63	[130-132,146]
2-ethyl phenol	c	-1044.07	-49.92	[148]
3-ethyl phenol	c	-1042.77	-51.22	[148]
4-ethyl phenol	c	-1040.35	-53.64	[148]

Aliphatic Di- and Polyols

Compound	State	ΔH_c° , 298°K kcal mol ⁻¹	ΔH_f° , 298°K kcal mol ⁻¹	Reference
1,2-ethanediol (ethylene glycol)	liq	-284.35	-108.70	[98,137,149,150,151]
1,2-propanediol	liq	-435.8	-119.6	[150,152]
1,3-propanediol	liq	-431.0	-124.4	[152]
1,2,3-propanetriol (glycerol)	liq	-395.65	-159.76	[60,98,115,149,153]
1,2,3,4-meso-butanetetrol (meso-erythritol)	c	-500.22	-217.56	[60,98,102, 137,155,156]
pentaerythritol	c	-660.1	-220.0	[137,157]
xylitol	c	-612.8	-267.3	[158]
L-arabitol	c	-611.4	-268.7	[137]
D-mannitol	c	-722.97	-319.54	[59,60,98,102,137, 153,159-161]
dulcitol	c	-720.68	-321.83	[59,60,98,137, 153,161]
D-perseitol	c	-835.2	-369.7	[137]
D-gluco- α -heptite	c	-840.4	-364.5	[162]
1,10-decanediol	c	-1526.20	-165.78	[163]
dipentaerythritol	c	-1315.1	-375.9	[164]

Aldehydes

Compound	State	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	Reference
methanal	g	-134.4	-28.0	[165]
ethanal	g	-258.01	-39.72	[166,167]
ethanal	liq	-278.77	-45.96	[168-171]
1-propanal	liq	-434.1	-53.0	[170-172]
1-butanal	liq	-592.2	-57.3	[172,173]
1-pentanal	liq	-742	-70	[174]
5-hydroxy-1-pentanal	liq	-697.1	-114.7	[175]
paraldehyde	liq	-810.0	-164.2	[176-178]
heptanal	liq	-1062.2	-74.4	[118,173]
octanal	liq	-1218.9	-80.0	[179]
benzaldehyde	liq	-843.2	-20.0	[180,181]
salicylaldehyde	liq	-796.4	-66.9	[182-184]

Ketones

Compound	State	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	Reference
2-propanone	g	-435.32	-51.78	[32,185]
2-propanone	liq	-427.92	59.18	[115,170,171, 186,187]
2-butanone	g	-590.20	-59.27	[188]
2-butanone	liq	-584.17	-65.30	[17,19,189-191]
2,3-butanedione	liq	-493.71	-87.44	[135,192-194]
3-pentanone	liq	-736.5	-75.3	[17,120,168,195]
acetophenone	liq	-991.60	-34.07	[196-199]
benzophenone	c	-1556.2	-8.0	[77,78,127, 198-201]

n-Aliphatic Acids

Compound	State	ΔH_c° , 298°K kcal mol ⁻¹	ΔH_f° , 298°K kcal mol ⁻¹	Reference
methanoic acid (formic acid)	liq	-60.86	-101.51	[113,114,202-205]
ethanoic acid (acetic acid)	liq	-209.02	-115.71	[113,114,205-210]
propanoic acid (propionic acid)	liq	-365.03	-122.07	[209,205,211-213]
n-butanoic acid (n-butyric acid)	liq	-521.87	-127.59	[205,212,213]
n-pentanoic acid (n-valeric acid)	liq	-678.12	-133.71	[205,212-215]
n-hexanoic acid (n-caproic acid)	liq	-834.49	-139.71	[66,128,205,214]
n-heptanoic acid (enanthic acid)	liq	-990.81	-145.75	[205,214]
n-octanoic acid (caprylic acid)	liq	-1147.00	-151.93	[205,214,216,217]
n-nonanoic acid (pelargonic acid)	liq	-1303.62	-157.67	[205,212-214,216,217]
n-decanoic acid (capric acid)	liq	-1460.10	-163.56	[214,222]
n-decanoic acid (capric acid)	c	-1453.07	-170.59	[60,153,212-214]
n-dodecanoic acid (lauric acid)	liq	-1772.02	-176.37	[214,222]
n-dodecanoic acid (lauric acid)	c	-1763.25	-185.14	[154,214-219]
n-tetradecanoic acid (myristic acid)	liq	-2084.59	-188.53	[214,222]
n-tetradecanoic acid (myristic acid)	c	-2073.91	-199.21	[59,60,153,154, 214,216-218,220]
n-hexadecanoic acid (palmitic acid)	liq	-2397.52	-200.34	[205,215,222]
n-hexadecanoic acid (palmitic acid)	c	-2384.76	-213.10	[60,115,205,212,213, 214,216,217,220]

n-Aliphatic Acids
(continued)

Compound	State	$\Delta H_{\text{c}}^{\circ}, 298^{\circ}\text{K}$ kcal mol ⁻¹	$\Delta H_{\text{f}}^{\circ}, 298^{\circ}\text{K}$ kcal mol ⁻¹	Reference
n-octadecanoic acid (stearic acid)	liq	-2710.12	-212.47	[205,214,222]
n-octadecanoic acid (stearic acid)	c	-2696.12	-226.47	[59,60,62,115,153,205, 212-214,217,220,221]
n-eicosanoic acid (arachidic acid)	liq	-3022.71	-224.61	[214,222]
n-eicosanoic acid (arachidic acid)	c	-3005.50	-241.82	[212-214]
n-docosanoic acid (behenic acid)	c	-3337.3	-234.8	[154]

Hydroxy Aliphatic Acids

Compound	State	ΔH_c° , 298°K kcal mol ⁻¹	ΔH_f° , 298°K kcal mol ⁻¹	Reference
glycolic acid (hydroxyacetic acid)	c	-166.1	-158.6	[102,223]
glyoxylic acid (dihydroxyacetic acid)	c	-125.0	-199.7	[202,224]
D-lactic acid	c	-321.22	-165.86	[225]
DL-lactic acid	c	-326.8	-160.3	[115,223]
mesoxalic acid	c	-128.1	-290.7	[226]
DL- β -hydroxybutyric acid	liq	-487.2	-162.3	[115]
hydroxyisobutyric acid	c	-471.6	-177.9	[223,227]
levulinic acid (4-ketovaleric acid)	c	-576.9	-166.6	[228]
D-gluconic acid	c	-594.9	-379.3	[229]
D-galactonic acid	c	589.4	-384.8	[229]
dihydroxybehenic acid	c	-3235.3	-336.8	[154]

Unsaturated Aliphatic Acids

Compound	State	ΔH_c° , 298°K kcal mol ⁻¹	ΔH_f° , 298°K kcal mol ⁻¹	Reference
acrylic acid	liq	-327.0	-91.8	[67,230]
cis-crotonic acid	liq	-498	-83	[231]
trans-crotonic acid	c	-478.2	-102.9	[199]
tiglic acid (cis- α,β -dimethylacrylic acid)	c	-626.2	-117.3	[199,232]
angelic acid (trans- α,β -dimethylacrylic acid)	c	-634.6	-108.9	[199,232]
sorbic acid	c	-744.2	-93.4	[66,199,233]
hydrosorbic acid	liq	-795.7	-110.2	
undecylenic acid	c	-1579.6	-138.1	[199]
oleic acid	liq	-2675.4	-178.9	[234]
oleic acid	c	-2667.1	-187.2	[115,199,234-236]
elaidic acid	c	-2636.6	-217.7	[199,234,235]
erucic acid	c	-3297.2	-206.5	[154,232]
brassicidic acid	c	-3290.1	-213.6	[154,232]

III. Selection of the Combustion Data

Aliphatic Hydrocarbons

The heats of combustion and formation of the selected values for the aliphatic hydrocarbons are the same as those found in reference [1].

methane - The combustion data of Rossini [2,3] were used to make the selection. The early studies on the heat of combustion of methane by Andrews [240], Favre and Silbermann [237], Thomsen [32,243] and Berthelot [244] are of historical interest only.

ethane - The combustion data of Rossini [4] were used to make the selection. The early studies by Thomsen [32], and Berthelot and Matignon [245] are of historical interest only.

propane - The combustion data of Rossini [4] were used to make the selection. The early studies of Thomsen [32], and Berthelot and Matignon [245] are of historical interest only.

n-pentane (g) - The combustion data of Rossini [4] were used to make the selection. The more recent data of Pilcher and Chadwick [143] are in very good agreement with the selection.

n-pentane (liq) - The combustion data of Prosen and Rossini [5] were used for the selected value. The recent data of Good [248] are in very good agreement with the selection. The earlier work of Roth and Macheleidt [246] was not used.

ethylene - The combustion data Rossini and Knowlton [6], and the heat-of-hydrogenation data of Kistiakowsky, Romeyn, Ruhoff, Smith, and Vaughan [7] as corrected by Prosen and Rossini [249] were used to obtain the selected value. The early studies of Dulong [250], Grassi [251], Favre and Silbermann [237], Andrews [242], Berthelot [244], Berthelot and Matignon [245], Thomsen [32], and Mixter [252] are of historical interest only.

acetylene - The unpublished combustion data of Prosen and Rossini cited in Wagman, Kilpatrick, Pitzer, and Rossini [8] were chosen for the selected value. The early studies of Thomsen [32], Berthelot [33, 244], Berthelot and Matignon [245], and Mixter [252] are of historical interest only.

Alicyclic Hydrocarbons

The selected values for the heats of combustion and formation of the alicyclic hydrocarbons are the same as those found in reference [1].

cyclopropane - The combustion data of Knowlton and Rossini [9] were chosen in preference to the earlier work by Berthelot [244], and Berthelot and Matignon [245,253].

cyclopentane - The combustion data of Johnson, Prosen, and Rossini [13] were used in preference to the data of Kaarsemaker and Coops [10], and Spitzer and Huffman [12]. The work of Zubov [254] as corrected by Swietoslawski [17] is of historical interest only.

cyclohexane - The combustion data of Good and Smith [20] and Johnson, Prosen, and Rossini [13] were used to make the selection. The data of Kaarsemaker and Coops [10], Spitzer and Huffman [12], and Moore, Renquist and Parks [19] were in good agreement with the selection. The works of Stohmann and Langbein [14,15], Zubov [16] as corrected by Swietoslawski [17], Roth and von Auwers [18] are of historical interest only.

cycloheptane - The combustion data of Spitzer and Huffman [12] and Kaarsemaker and Coops [10] were averaged to obtain the selected value. The data of Zubov [16] as corrected by Swietoslawski [17] was not used.

cyclooctane - The combustion data of Kaarsemaker and Coops [10], and Spitzer and Huffman [12] were averaged to obtain the selected value. The data of Schläpfer [21] and Ruzicka and Schläpfer [22] were not used.

Aromatic Hydrocarbons

benzene (g) - References [23] to [30] provided experimental data on the determination of the heat of vaporization of benzene. We have used the ideal heat of vaporization at 25°C of $8.10 \text{ kcal mol}^{-1}$ as in reference [1]. By combining the latter value with the $\Delta H_{\text{c}}^{\circ}[\text{C}_6\text{H}_6(\text{liq})] = -780.96 \text{ kcal mol}^{-1}$, we calculate $\Delta H_{\text{c}}^{\circ} = -789.06 \text{ kcal mol}^{-1}$ for gaseous benzene. The early studies on the heat of combustion of gaseous benzene, references [32] to [37] were not used and are of historical interest only.

benzene (liq) - The combustion data of Good and Smith [20], and Prosen, Gilmont, and Rossini [47] were used to obtain the selected value. The data of Coops, Mulder, Dienske, and Smittenberg [45,46] were not used. References [38] to [44] summarize the early studies, and are of historical interest only.

naphthalene (g) - The sublimation pressures of naphthalene were measured by Bradley and Cleasby [48], Sherwood and Bryant [49], Miller [50], Zil'berman-Granovskaya [51], Swan and Mack [52], Winstrom and Kulp [53], Allen [54], Hoyer and Peperle [55], Aihara [56], Sears and Hopke [57], and Shlyarenko, Martin, and Belyaeva [58]. When plotted individually as $\log P$ vs $1/T$, these sets of data show generally poor agreement, but when considered as a whole, good agreement results, giving a reasonably straight line. Using a least squares treatment of the vapor pressure data, we obtain for the heat of sublimation, $17.6 \text{ kcal mol}^{-1}$ at 25°C. Combining this with our selection, $\Delta H_{\text{c}}^{\circ}[\text{C}_{10}\text{H}_8(\text{c})] = -1231.8 \text{ kcal mol}^{-1}$, we calculate $\Delta H_{\text{c}}^{\circ} = -1249.4 \text{ kcal mol}^{-1}$ for gaseous naphthalene.

naphthalene (c) - The heat of combustion of naphthalene (c) was measured by von Rechenberg [59], Stohmann [60,61], Rübner [62], Berthelot and Louguinine [63], Berthelot and Recoura [64], Berthelot and Vieille [65], Fischer and Wrede [66], Riiber and Schetelig [67], Wrede [68], Dickinson [69], Karrar and Fioroni [71], Verkade and Coops [75,76], Beckers [77], Burriel [78], Keffler [79], Milone and Rossignoli [80], Schläpfer and Fioroni [81], Huffman and Ellis [82], Bender and Farber [83], Speros and Rossini [84], Prosen and Colomina [85], Mackle and O'Hare [86], and Coleman and Pilcher [87]. The value for the heat of combustion of naphthalene relative to that of benzoic acid was well-established by various experimenters as 1.5202 to 1.5204. For a discussion of this point see Verkade [74], Verkade, Coops and Hartman [73], Swietoslowski [70], and Swietoslowski and Starczewska [72]. If we take the value 1.5204, and the presently accepted value for benzoic acid ($-\Delta U_p = 26434 \text{ Jg}^{-1}$ (vacuum) at 25°C), and apply the appropriate corrections (for standard state condition, ΔnRT and calculation of ΔH_f°), we obtain for our selected values $\Delta H_c^\circ = -1231.8 \text{ kcal mol}^{-1}$, and $\Delta H_f^\circ = +18.0 \text{ kcal mol}^{-1}$.

anthracene (g) - Sublimation pressures have been measured by Bradley and Cheasby [48], Stevens [88], Klochkov [89], Inokuchi, Shiba, Handa, and Akamatu [90], Sears and Hopke [57], Nitta, Seki, and Momotani [91], Kelly and Rice [92], and Hoyer and Peperle [55]. As a result of examining the experimental data, we obtained a selected heat of sublimation of $24.7 \text{ kcal mol}^{-1}$. By combining the latter with $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1687.3 \text{ kcal mol}^{-1}$, we calculate $\Delta H_c^\circ = -1714.7 \text{ kcal mol}^{-1}$ for gaseous anthracene.

anthracene (c) - The heat of combustion of anthracene (c) was measured by von Rechenberg [59], Stohmann [60], Stohmann, Kleber, and Langbein [38], Berthelot and Vieille [65,100], Beckers [77], Burriel [78], Wiegert [93], Klaproth [94], Milone and Rossignoli [80], Fries, Walter, and Schilling [95], Shchukarev and Shchukareva [96], Richardson and Parks [97], Parks, West, Naylor, Fugii, and McClaine [98], Bender and Farber [83], Magnus, Hartmann, and Becker [99], Mackle and O'Hare [86], and Coleman and Pilcher [87]. An average heat of combustion derived from the data of the last six investigations [83,86,87,97,98,99], mentioned constitutes our selected value. $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1687.3 \text{ kcal mol}^{-1}$.

phenanthrene (g) - Sublimation pressures were measured by Bradley and Cleasby [48], Inokuchi, Shiba, Handa, and Akamatu [90], and Hoyer and Peperle [55]. From these data we derived the heat of sublimation at 25°C of $21.1 \text{ kcal mol}^{-1}$ from the data of Bradley and Cleasby [48]. By combining $\Delta H(\text{sublimation})$ with $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1685.6 \text{ kcal mol}^{-1}$, we calculate $\Delta H_c^\circ = -1706.7 \text{ kcal mol}^{-1}$ for gaseous phenanthrene.

phenanthrene (c) - The heat of combustion of phenanthrene (c) was measured by Stohmann, Kleber, and Langbein [38], Berthelot and Vieille [65,100], Klaproth [94], Milone and Rossignoli [80], Shchukarev and Shchukareva [96], Fries, Walter, and Schilling [95], Richardson and Parks [97], Bender and Farber [83], Magnus, Hartmann and Becker [99], and Coleman and Pilcher [87]. An average heat of combustion derived from the data of the last three investigations [83,87,99], mentioned constitutes our selected value. $\Delta H_c^\circ[\text{C}_{14}\text{H}_{10}(\text{c})] = -1685.6 \text{ kcal mol}^{-1}$.

pyrene - The combustion data of Westrum and Wong [101] were preferred to that of Richardson and Parks [97] in making the selection.

triphenylene - The combustion data of Westrum and Wong [101] were preferred to that of Magnus, Hartmann, and Becker [99] in making the selection.

chrysene - The combustion data of Magnus, Hartmann, and Becker [99] were preferred to that of Stohmann [102] in making the selection.

perylene - The combustion data of Westrum and Wong [101] were preferred to that of Pongratz, and Griengl [103] in making the selection.

fluoranthrene - The combustion data of Westrum and Wong [101], and Boyd, Christensen, and Pua [104] were averaged in obtaining the selected value.

Aliphatic Alcohols

methanol (g) - The combustion data of Rossini [105] on gaseous methanol were chosen in preference to the early work of Thomsen [32]. The data of Favre and Silbermann [237] are of historical interest only. The heat of vaporization of methanol at 25°C was taken from the measurements of Fiock, Ginnings, and Holton [239], ΔH_{vap} at 25°C = 8.95 kcal mol⁻¹. Recent vaporization data by Wadsbø [112] are in very good agreement with the data of Fiock, Ginnings, and Holton [239]. A correction for dimer and tetramer formation was made to the vaporization data using the study of Weltner and Pitzer [238], amounting to 0.13 kcal mol⁻¹. This gives ΔH_{vap} at 25°C = 9.08 kcal mol⁻¹ for the process: $\text{CH}_3\text{OH}(\text{liq}) = \text{CH}_3\text{OH}(\text{g}, \text{monomer})$.

methanol (liq) - Our selected value for the heat of combustion of $\text{CH}_3\text{OH}(\text{liq})$ is obtained by combining the value for the heat of combustion of $\text{CH}_3\text{OH}(\text{g})$ with the heat of vaporization of the liquid to the gaseous monomer. The recent data of Chao and Rossini [111] is in good agreement with our selection. The earlier work of Stohmann,

Kleber, and Langbein [106], Richards and Davis [42], Roth [107], Roth and Banse [108], Roth and Müller [109] and I. G. Farbenfabriken [110] has not been used.

ethanol (g) - The combustion data of Rossini [105] on gaseous ethanol were chosen in preference to the earlier data of Thomsen [32]. The data of Andrews [240] and Favre and Silbermann [237] are only of historical interest. The heat of vaporization of ethanol at 25°C was taken from the measurements of Fiock, Ginnings, and Holton [239], ΔH_{vap} at 25°C = 10.13 kcal mol⁻¹. Recent vaporization data by Wadsbø [112] are in very good agreement with the data of Fiock, Ginnings, and Holton [239]. A correction for the presence of dimeric ethanol (g) was introduced from the data of Coburn, and Grunwald [241] amounting to 0.05 kcal mol⁻¹. Hence, for the process: $\text{CH}_3\text{CH}_2\text{OH}(\text{liq}) = \text{CH}_3\text{CH}_2\text{OH}(\text{g, monomer})$, ΔH_{vap} at 25°C = 10.18 kcal mol⁻¹.

ethanol (liq) - Our selection for the heat of combustion was obtained by combining, the value for the heat of combustion of $\text{CH}_3\text{CH}_2\text{OH}(\text{g})$ with the heat of vaporization of the liquid to the gaseous monomer. The recent data of Chao and Rossini [111] are in good agreement with our selection. The earlier data of Berthelot and Matignon [113,114], Emery and Benedict [115], Atwater and Rosa [116], Atwater and Snell [117], Roth and Muller [109] and Richards and Davis [42] were not used.

1-propanol - The combustion data of Chao and Rossini [111] and Snelson and Skinner [119] were averaged to obtain the selected value. The earlier data were not used.

2-propanol - The combustion data of Chao and Rossini [111], Snelson and Skinner [119], and Parks, Mosley and Peterson [190] were averaged to obtain the selected value. The earlier data were not used.

1-butanol - The combustion data of Verkade and Coops [123], Chao and Rossini [111], Skinner and Snelson [121], Mosselman and Dekker [247], and Gundry, Head, and Lewis [122] were averaged to obtain the selected value. The early data of Zubov [120] and the correction of the latter by Swietoslowski [17] was not used. The combustion data of Tjebbes [124] appeared not negative enough by at least one kilocalorie per mole, and hence, were not used.

2-butanol - The combustion data of Chao and Rossini [111], and Skinner and Snelson [121] were averaged to obtain the selection.

2-methyl-1-propanol - The combustion data of Chao and Rossini [111] and Skinner and Snelson [121] were averaged to obtain the selected value. The earlier data was not used.

1-pentanol - The combustion data of Verkade and Coops [123], Chao and Rossini [111], and Gundry, Harrop, Head, and Lewis [125] were averaged to obtain the selected value. The earlier data were not used.

1-hexanol - The combustion data of Verkade and Coops [123], and Chao and Rossini [111], were averaged to obtain the selected value.

Phenols

phenol - The heat of combustion of phenol was measured by von Rechenberg [59], Stohmann [60,102] Berthelot and Louguinine [63], Berthelot and Vieille [65], Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [130], Cox [131,132], Karlsson [133], Manchester [134], Parks, Manchester, and Vaughan [135], Stohmann, Rodatz, and Herzberg [136], Stohmann and Langbein [137], and Badoche [138]. We have used the data of Andon, et al. [130] for our selected value.

pyrocatechol - The combustion data of Stohmann [102], and Stohmann and Langbein [137] were obtained using an oxygen bomb calorimeter, and are preferred to the data of Stohmann [60] in which the potassium chlorate-oxidative mixture technique was used. The data in references [102] and [137] are the same. The heat of combustion calculated from the latter was found to be $-684.9 \text{ kcal mol}^{-1}$ after all corrections were applied. This was reduced to $-683.0 \text{ kcal mol}^{-1}$ because the value for the heat of combustion of phenol found by Stohmann and Langbein was 2 to 3 kcal mol^{-1} more negative than our presently selected value for phenol.

resorcinol - The combustion data of Desai, Wilhoit, and Zwolinski [139] was chosen in preference to the earlier combustion data.

hydroquinone - The combustion data of Pilcher and Sutton [142] was chosen in preference to any other combustion data.

o-cresol - The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [130], and Cox [131,132] were chosen in preference to the data of Stohmann, Rodatz, and Herzberg [146].

m-cresol - The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [130], and Cox [131,132] were chosen in preference to the earlier data.

p-cresol - The combustion data of Andon, Biddiscombe, Cox, Handley, Harrop, Herington, and Martin [130], and Cox [131,132] were chosen in preference to the data of Stohmann, Rodatz and Herzberg [146].

Aliphatic Di- and Polyols

1,2-ethanediol, (ethylene glycol) - The combustion data of Parks, West, Naylor, Fujii, and McClaine [98] were preferred for the selected value to the earlier data.

1,2-propanediol - The combustion data of Moureu and Dode [150] were preferred to that of Louguinine [152].

1,2,3-propenetriol, (glycerol) - The combustion data of Parks, West, Naylor, Fujii, and McClaine [98] were chosen in preference to the earlier combustion data.

1,2,3,4-meso-butanetetrol, (meso-erythritol) - The combustion data of Parks, West, Naylor, Fujii, and McClaine [98] were chosen in preference to the earlier combustion data.

pentaerythritol - The combustion data of Medard and Thomas [157] were preferred to the data of Stohmann [137].

D-mannitol - The combustion data of Parks, West, Naylor, Fujii and McClaine [98] were preferred to any data published before 1900 (references [59,60,102,137,153,159,161]). The recent combustion data of Baer and Flehmig [160] are in poor agreement with our selected value by 6 to 7 kcal mol⁻¹. Details of their calorimetric data are scant, and the 6 to 7 kcal mol⁻¹ could be the overall uncertainty in the experiment.

dulcitol - The combustion data of Parks, West, Naylor, Fujii, and McClaine [98] were chosen in preference to the earlier combustion data.

Aldehydes

ethanal (g) - The heat-of-hydrogenation data of Dolliver, Gresham, Kistiakowsky, Smith, and Vaughan [167] was used as the basis of our selected value rather than the early combustion of Berthelot and Ogier [166].

ethanal (liq) - The heat of vaporization of ethanal as determined by Coleman and DeVries [169], $6.24 \text{ kcal mol}^{-1}$ at 25°C , was combined with the heat of formation of gaseous ethanal. The combustion data of Berthelot and Delepine [170,171], and Roth and Miller [168] was not used.

1-propanal - The combustion data of Tjebbes [172] were used to obtain the selection. The data of Berthelot and Delepine [170,171] were not used.

1-butanal - The combustion data of Tjebbes [172] and Nicholson [173] were averaged to make the selection.

paraaldehyde - The combustion data of Fletcher, Mortimer, and Springall [178] were used to obtain the selected value. The same data are given earlier by Cass, Springall, and White [177], but show ΔH_c° to be more negative by $0.2 \text{ kcal mol}^{-1}$. The combustion data of Louguinine [176] were not used.

heptanal - The combustion data of Nicholson [173] were chosen in preference to the data of Louguinine [118].

benzaldehyde - The combustion data of Landrieu, Baylocq, and Johnson [180] were chosen in preference to the data of Stohmann, Rodatz, and Herzberg [181].

salicylaldehyde - The combustion data of Delepine and Rivals [182] were chosen in preference to the data of Berthelot and Rivals [183] and Rivals [184].

Ketones

2-propanone (g) - The combustion data of Miles and Hunt [185] were chosen in preference to the early data of Thomsen [32].

2-propanone (liq) - The heat of vaporization was taken from the data of Pennington and Kobe [187], $\Delta H_{\text{vap}}^{\circ}$ at 25°C = 7.40 kcal mol⁻¹. The latter value was combined with the heat of combustion of gaseous 2-propanone. The combustion data of Berthelot and Delepine [170,171], Emery and Benedict [115], and Taylor, Hall, and Thomas [186] were not used.

2-butanone (liq) - The combustion data of Sinke and Oetting [191] were chosen in preference to any previous work.

2,3-butanedione - The combustion data of Nicholson, Szwarc, and Taylor [193], and Parks, Manchester, and Vaughan [135] were averaged to make the selection. The data of Springall and White [194] and Landrieu [192] were not used.

3-pentanone - The combustion data of Roth and Miller [168] and Louguinine [195] were averaged to obtain the selected value. The data of Zubov [120] as corrected by Swietoslawski [17] were not used.

acetophenone - The combustion data of Colomina, Latorre, and Perez-Ossorio [196,197] were chosen in preference to the early combustion data of Stohmann [199], and Stohmann, Rodatz, and Herzberg [198].

benzophenone - The combustion data of Colomina, Cambeiro, Perez-Ossorio, and Latorre [200], and Parks, Mosley, and Peterson [127] were averaged for the selection. The data of Beckers [77], Burriel [78], Landrieu, and Blatt [201], Stohmann, Rodatz, and Herzberg [198], and Stohmann [199] were not used.

n-Aliphatic Acids

methanoic acid, (formic acid) - The combustion data of Sinke [204] were used to obtain the selected value. The data of Lebedeva [205] are in excellent agreement with the selection. The data of Berthelot [202], Berthelot and Matignon [113,114], and Jahn [203] were not used.

ethanoic acid, (acetic acid) - The combustion data of Evans and Skinner [206] were used to obtain the selected value. The data of Lebedeva [205] are in excellent agreement with the selection. The data of Berthelot and Matignon [113,114], Roth [207], Schjanberg [208,209] and Stull [210] were not used, although only the data of Roth [207] appeared to deviate from the selection by more than $0.3 \text{ kcal mol}^{-1}$.

propanoic acid, (propionic acid) - The combustion data of Lebedeva [205] were chosen in preference to the previous data.

n-butanoic acid, (n-butyric acid) - The combustion data of Lebedeva [205] were chosen in preference to the early data.

n-pentanoic acid, (n-valeric acid) - The combustion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selected value. The data of Hancock, Watson, and Gilby [215] agree well with the early work of Stohmann, Kleber, Langbein, and Offenbauer [212,213]. Data from the latter three references were not used.

n-hexanoic acid, (n-caproic acid) - The combustion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selected value. The data of Fischer and Wrede [66], and Louguinine [128] were not used.

n-heptanoic acid, (enanthic acid) - The combustion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selection.

n-octanoic acid, (caprylic acid) - The combustion data of Lebedeva [205] and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selected value. The data of Louguinine [216,217] were not used.

n-nonanoic acid, (pelargonic acid) - The combustion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selection. The early data [212,213,216,217] were not used.

n-decanoic acid, (capric acid)(c) - The combustion data of Adriaanse, Dekker, and Coops [214] were chosen in preference to the earlier data.

n-dodecanoic acid, (lauric acid)(c) - The combustion data of Adriaanse, Dekker, and Coops [214] were chosen in preference to the earlier data.

n-tetradecanoic acid, (myristic acid)(c) - The combustion data of Adriaanse, Dekker, and Coops [214] was used to obtain the selected value. The data of Swain, Silbert, and Miller [220], although not as precise, are in good agreement with the selection. The early combustion data [59,60,153,154,216,217,218] were not used.

n-hexadecanoic acid, (palmitic acid)(liq) - The heat of fusion as determined by Adriaanse, Dekker, and Coops [214,222] was selected in preference to the data of Lebedeva [205].

n-hexadecanoic acid, (palmitic acid)(c) - The combustion data of Adriaanse, Dekker, and Coops [214] were used to obtain the selected value in preference to the data of Lebedeva [205]. The data of Swain, Silbert, and Miller [220], although not as precise as either of the above data is in good agreement with the data of Adriaanse, Dekker and Coops [214]. Data prior to the above [60,115,212,213, 216,217] were not used.

n-octadecanoic acid, (stearic acid)(liq) - The fusion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214,222] were averaged to obtain the selected value, $\Delta H(\text{fusion})$ at $25^\circ\text{C} = 14.0 \text{ kcal mol}^{-1}$.

n-octadecanoic acid, (stearic acid)(c) - The combustion data of Lebedeva [205], and Adriaanse, Dekker, and Coops [214] were averaged to obtain the selected value. The combustion data of Swain, Silbert, and Miller [220] are too positive by about $2.2 \text{ kcal mol}^{-1}$. Data prior to the above [59,60,62,115,153,212,213,217,221] were not used.

n-eicosanoic acid, (arachidic acid)(c) - The combustion data of Adriaanse, Dekker, and Coops [214] were preferred to the earlier work.

Hydroxy Aliphatic Acids

glycolic acid, (hydroxyacetic acid) - The combustion data of Louguinine [223], and Stohmann [102] were averaged to obtain the selected value.

glyoxylic acid, (dihydroxyacetic acid) - The combustion data of Berthelot [202] are the same as Berthelot and Matignon [224].

DL-lactic acid - The combustion data of Emery and Benedict [115] and Louguinine [223] were averaged to obtain the selected value.

hydroxyisobutyric acid - The later combustion data of Louguinine [223] was preferred to the earlier work by the same author [227].

Unsaturated Aliphatic Acids

acrylic acid - The combustion data of Moureu and Boutaric [230], and Riiber and Schetelig [67] were averaged to obtain the selected value.

tiglic acid - The combustion data of Stohmann [199] and Stohmann [232] are the same.

angelic acid - The combustion data of Stohmann [199] and Stohmann [232] are the same.

sorbic acid - The combustion data of Fischer and Wrede [66] were chosen in preference to the data of Stohmann [199] and Osipov [233].

oleic acid (c) - The combustion data of Keffler and McLean [236] were chosen in preference to previous data.

elaidic acid - The combustion data of Keffler [234,235] were chosen in preference to the data of Stohmann [199].

erucic acid - The combustion data of Stohmann and Langbein [154] are the same as Stohmann [232].

brassicidic acid - The combustion data of Stohmann and Langbein [154] are the same as Stohmann [232].

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