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NATIONAL BUREAU OF STANDARDS REPORT

9883

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

Progress Report for the Period 1 March to 30 June 1968

to

National Aeronautics and Space Administration

22 July 1968



U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

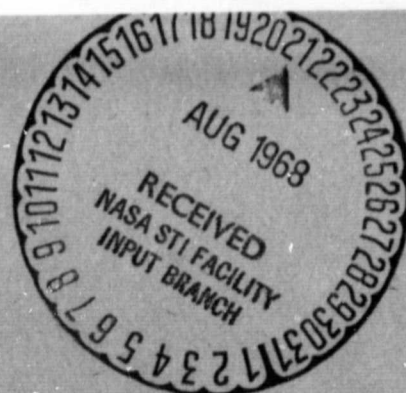
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NBS REPORT

9883

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

George T. Furukawa, Martin L. Reilly,
and Eugene S. Domalski

Progress Report for the Period 1 March to 30 June 1968
to
National Aeronautics and Space Administration
Contract No. R-138, Amendment 3

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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 fourteenth 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 account 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 prebiological 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 Heat Division, Institute for Basic Standards (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended by Amendments 1, 2, and 3. This report covers a portion of the work under Amendment 3. 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.

George T. Armstrong

George T. Armstrong
Supervisory Chemist
Project Leader

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Section I.

Thermodynamic Properties of CHNOPS Compounds

G. T. Furukawa and M. L. Reilly

Tables of thermodynamic properties have been calculated for twelve additional substances in their ideal-gas state using statistical methods. The molecular constants and the spectroscopic data used for the substances are those given in the JANAF Tables. The value used for the gas constant R is 8.3143/4.1840 cal/K-mol accepted by the National Bureau of Standards. The 1961 atomic weights based on C-12 were used in the calculations.

The values of thermodynamic properties calculated using the molecular constants and spectroscopic data have been compared with those given in the JANAF Tables. It seems that the gram-formula-weight used for C_2^- in the JANAF Tables is for C_2^+ . The JANAF Table values for CCH are not consistent with their March 31, 1967 values of molecular and spectroscopic data. The table values correspond with their older December 31, 1966 values of spectroscopic and molecular data. The thermodynamic properties given in this report are based on their March 31, 1967 values of molecular and spectroscopic data.

LIST OF THERMODYNAMIC TABLES OF CHNOPS COMPOUNDS

<u>Table</u>	<u>Compound</u>	<u>State</u>
131	Formyl Unipositive Ion (CHO^+)	Ideal gas
132	CNN Radical (CN_2)	Ideal gas
133	NCN Radical (CN_2)	Ideal gas
134	Carbon Dioxide Uninegative Ion (CO_2^-)	Ideal gas
135	Dimeric Carbon Uninegative Ion (C_2^-)	Ideal gas
136	CCH Radical (C_2H)	Ideal gas
137	CNC Radical (C_2N)	Ideal gas
138	CCO Radical (C_2O)	Ideal gas
139	Proton (H^+)	Ideal gas
140	Nitric Oxide Unipositive Ion (NO^+)	Ideal gas
141	Phosphorus Nitride (NP)	Ideal gas
142	Diatomic Oxygen Uninegative Ion (O_2^-)	Ideal gas

TABLE 131

MOLAL THERMODYNAMIC PROPERTIES FOR FORMYL UNIPOSITIVE ION (CHO^+)

IDEAL GAS

GRAM FORMULA WT. = 29.01797 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_P^0 --K-- --CAL-- --MOL--	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ --K-- --CAL-- --MOL--	S_T^0 --K-- --CAL-- --MOL--	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ --K-- --CAL-- --MOL--
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	6.972	694.19	6.942	40.135	3319.3	33.193
200.00	7.619	1415.7	7.079	45.111	7606.4	38.032
273.15	8.380	2001.1	7.326	47.599	11000.	40.273
298.15	8.617	2213.6	7.425	48.343	12199.	40.919
300.00	8.634	2229.6	7.432	48.397	12289.	40.965
373.15	9.216	2883.4	7.727	50.344	15902.	42.617
400.00	9.393	3133.2	7.833	50.991	17263.	43.158
500.00	9.942	4101.2	8.202	53.149	22473.	44.946
600.00	10.385	5118.2	8.530	55.002	27882.	46.471
700.00	10.777	6176.6	8.824	56.632	33466.	47.809
800.00	11.138	7272.6	9.091	58.095	39203.	49.005
900.00	11.472	8403.3	9.337	59.427	45080.	50.090
1000.00	11.781	9566.2	9.566	60.652	51085.	51.086
1100.00	12.064	10758.	9.781	61.788	57208.	52.007
1200.00	12.320	11978.	9.982	62.849	63440.	52.867
1300.00	12.552	13221.	10.171	63.844	69775.	53.674
1400.00	12.760	14487.	10.348	64.782	76207.	54.434
1500.00	12.946	15773.	10.515	65.669	82730.	55.154
1600.00	13.113	17076.	10.673	66.510	89339.	55.837
1700.00	13.262	18395.	10.821	67.310	96031.	56.489
1800.00	13.395	19728.	10.960	68.072	102800.	57.111
1900.00	13.515	21073.	11.091	68.799	109644.	57.708
2000.00	13.622	22430.	11.215	69.495	116559.	58.280
2100.00	13.718	23797.	11.332	70.162	123542.	58.830
2200.00	13.804	25173.	11.443	70.802	130590.	59.359
2300.00	13.882	26558.	11.547	71.418	137702.	59.870
2400.00	13.953	27950.	11.646	72.010	144873.	60.364
2500.00	14.017	29348.	11.739	72.581	152103.	60.841
2600.00	14.075	30753.	11.828	73.132	159389.	61.303
2700.00	14.127	32163.	11.912	73.664	166729.	61.751
2800.00	14.175	33578.	11.992	74.179	174121.	62.186
2900.00	14.219	34998.	12.068	74.677	181564.	62.608
3000.00	14.260	36422.	12.141	75.159	189056.	63.019
3100.00	14.296	37850.	12.210	75.628	196595.	63.418
3200.00	14.330	39281.	12.275	76.082	204181.	63.807
3300.00	14.362	40716.	12.338	76.524	211811.	64.185
3400.00	14.390	42153.	12.398	76.953	219485.	64.555
3500.00	14.417	43594.	12.455	77.370	227201.	64.915
3600.00	14.442	45037.	12.510	77.777	234959.	65.266
3700.00	14.465	46482.	12.563	78.173	242756.	65.610
3800.00	14.486	47930.	12.613	78.559	250593.	65.946
3900.00	14.506	49379.	12.661	78.935	258468.	66.274
4000.00	14.524	50831.	12.708	79.303	266380.	66.595
4100.00	14.541	52284.	12.752	79.662	274328.	66.909
4200.00	14.558	53739.	12.795	80.012	282312.	67.217
4300.00	14.573	55195.	12.836	80.355	290330.	67.519
4400.00	14.587	56653.	12.876	80.690	298382.	67.814
4500.00	14.600	58113.	12.914	81.018	306468.	68.104
4600.00	14.612	59573.	12.951	81.339	314586.	68.388
4700.00	14.624	61035.	12.986	81.654	322736.	68.667
4800.00	14.635	62498.	13.021	81.962	330916.	68.941
4900.00	14.646	63962.	13.054	82.263	339128.	69.210
5000.00	14.655	65427.	13.086	82.559	347369.	69.474
5100.00	14.665	66893.	13.116	82.850	355639.	69.733
5200.00	14.673	68360.	13.146	83.135	363939.	69.988
5300.00	14.682	69828.	13.175	83.414	372266.	70.239
5400.00	14.690	71297.	13.203	83.689	380621.	70.486
5500.00	14.697	72766.	13.230	83.958	389004.	70.728
5600.00	14.704	74236.	13.257	84.223	397413.	70.967
5700.00	14.711	75707.	13.282	84.483	405848.	71.202
5800.00	14.717	77178.	13.307	84.739	414309.	71.433
5900.00	14.723	78650.	13.331	84.991	422796.	71.660
6000.00	14.729	80123.	13.354	85.239	431307.	71.885

TABLE 132

MOLAL THERMODYNAMIC PROPERTIES FOR CNH RADICAL (CN₂)

IDEAL GAS

GRAM FORMULA WT. = 40.02455 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C _P -R CAL -MOL-	(H _T ⁰ -H ₀ ⁰) CAL MOL	(H _T ⁰ -H ₀ ⁰)/T -R CAL -MOL-	S _T ⁰ -R CAL -MOL-	-(G _T ⁰ -H ₀ ⁰) CAL MOL	-(G _T ⁰ -H ₀ ⁰)/T -R CAL -MOL-
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.403	702.97	7.030	45.836	3880.7	38.807
200.00	9.100	1532.4	7.662	51.516	8770.8	43.854
273.15	9.893	2229.0	8.160	54.478	12651.	46.318
298.15	10.105	2479.0	8.315	55.354	14024.	47.039
300.00	10.120	2497.7	8.326	55.416	14127.	47.091
373.15	10.639	3257.7	8.730	57.681	18266.	48.951
400.00	10.803	3545.6	8.864	58.426	19824.	49.562
500.00	11.323	4653.0	9.306	60.895	25794.	51.589
600.00	11.745	5807.0	9.678	62.998	31991.	53.320
700.00	12.104	6999.9	10.000	64.836	38385.	54.836
800.00	12.416	8226.2	10.283	66.473	44952.	56.190
900.00	12.691	9481.9	10.535	67.952	51674.	57.416
1000.00	12.933	10763.	10.763	69.302	58538.	58.538
1100.00	13.144	12067.	10.970	70.544	65531.	59.574
1200.00	13.330	13391.	11.159	71.696	72644.	60.537
1300.00	13.491	14732.	11.333	72.770	79868.	61.437
1400.00	13.633	16088.	11.492	73.775	87195.	62.283
1500.00	13.756	17458.	11.639	74.720	94621.	63.081
1600.00	13.864	18839.	11.775	75.611	102138.	63.836
1700.00	13.959	20230.	11.900	76.454	109741.	64.554
1800.00	14.042	21630.	12.017	77.255	117427.	65.237
1900.00	14.115	23038.	12.126	78.016	125191.	65.890
2000.00	14.180	24453.	12.227	78.742	133029.	66.515
2100.00	14.238	25874.	12.321	79.435	140938.	67.114
2200.00	14.290	27301.	12.410	80.098	148915.	67.689
2300.00	14.335	28732.	12.492	80.735	156957.	68.242
2400.00	14.377	30168.	12.570	81.346	165061.	68.776
2500.00	14.414	31607.	12.643	81.933	173225.	69.290
2600.00	14.447	33050.	12.712	82.499	181447.	69.787
2700.00	14.477	34496.	12.777	83.045	189724.	70.268
2800.00	14.505	35946.	12.838	83.572	198055.	70.734
2900.00	14.530	37397.	12.896	84.081	206438.	71.186
3000.00	14.552	38851.	12.951	84.574	214871.	71.624
3100.00	14.573	40308.	13.003	85.052	223352.	72.049
3200.00	14.592	41766.	13.052	85.515	231881.	72.463
3300.00	14.610	43226.	13.099	85.964	240455.	72.865
3400.00	14.626	44688.	13.144	86.401	249073.	73.257
3500.00	14.640	46151.	13.186	86.825	257735.	73.639
3600.00	14.654	47616.	13.227	87.237	266438.	74.011
3700.00	14.667	49082.	13.266	87.639	275182.	74.374
3800.00	14.678	50549.	13.303	88.030	283965.	74.728
3900.00	14.689	52018.	13.338	88.412	292788.	75.074
4000.00	14.699	53487.	13.372	88.784	301647.	75.412
4100.00	14.709	54958.	13.404	89.147	310544.	75.743
4200.00	14.718	56429.	13.436	89.502	319477.	76.066
4300.00	14.726	57901.	13.465	89.848	328444.	76.382
4400.00	14.734	59374.	13.494	90.187	337446.	76.692
4500.00	14.741	60848.	13.522	90.518	346481.	76.996
4600.00	14.748	62322.	13.548	90.842	355549.	77.293
4700.00	14.754	63797.	13.574	91.159	364649.	77.585
4800.00	14.760	65273.	13.599	91.470	373781.	77.871
4900.00	14.766	66749.	13.622	91.774	382943.	78.152
5000.00	14.771	68226.	13.645	92.072	392135.	78.427
5100.00	14.776	69703.	13.667	92.365	401357.	78.698
5200.00	14.781	71181.	13.689	92.652	410608.	78.963
5300.00	14.785	72660.	13.709	92.934	419888.	79.224
5400.00	14.789	74138.	13.729	93.210	429195.	79.481
5500.00	14.793	75617.	13.749	93.481	438529.	79.733
5600.00	14.797	77097.	13.767	93.748	447891.	79.981
5700.00	14.801	78577.	13.786	94.010	457279.	80.224
5800.00	14.804	80057.	13.803	94.267	466693.	80.464
5900.00	14.808	81538.	13.820	94.520	476122.	80.700
6000.00	14.811	83019.	13.837	94.769	485597.	80.933

TABLE 133

MOLAL THERMODYNAMIC PROPERTIES FOR NCN RADICAL (CN₂)

IDEAL GAS

GRAM FORMULA WT. = 40.07455 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_p^0 -R-MOL-	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ -R-MOL-	S_T^0 -R-MOL-	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ -R-MOL-
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.294	700.66	7.007	44.682	3767.6	37.676
200.00	9.098	1518.8	7.594	50.280	8537.1	42.686
273.15	10.201	2226.4	8.151	53.286	12328.	45.135
298.15	10.515	2485.5	8.336	54.193	13672.	45.857
300.00	10.537	2504.9	8.350	54.258	13772.	45.900
373.15	11.310	3305.1	8.857	56.642	17830.	47.789
400.00	11.551	3612.1	9.030	57.437	19362.	48.406
500.00	12.292	4806.1	9.612	60.098	25242.	50.486
600.00	12.840	6064.1	10.107	62.300	31369.	52.283
700.00	13.248	7369.4	10.528	64.401	37711.	53.873
800.00	13.555	8710.3	10.888	66.191	44242.	55.303
900.00	13.789	10078.	11.198	67.802	50943.	56.604
1000.00	13.970	11466.	11.466	69.264	57798.	57.798
1100.00	14.112	12870.	11.701	70.603	64792.	58.902
1200.00	14.225	14287.	11.906	71.836	71915.	59.929
1300.00	14.316	15715.	12.088	72.978	79156.	60.890
1400.00	14.391	17150.	12.250	74.042	86508.	61.792
1500.00	14.452	18592.	12.395	75.037	93962.	62.642
1600.00	14.504	20040.	12.525	75.971	101513.	63.446
1700.00	14.547	21493.	12.643	76.852	109155.	64.209
1800.00	14.583	22949.	12.750	77.685	116882.	64.935
1900.00	14.615	24409.	12.847	78.474	124690.	65.627
2000.00	14.642	25872.	12.936	79.224	132575.	66.288
2100.00	14.665	27337.	13.018	79.939	140534.	66.921
2200.00	14.686	28805.	13.093	80.622	148562.	67.528
2300.00	14.704	30275.	13.163	81.275	156657.	68.112
2400.00	14.719	31746.	13.228	81.901	164816.	68.674
2500.00	14.734	33218.	13.288	82.502	173037.	69.215
2600.00	14.746	34692.	13.343	83.081	181316.	69.737
2700.00	14.757	36168.	13.396	83.637	189652.	70.242
2800.00	14.767	37644.	13.444	84.174	198043.	70.730
2900.00	14.776	39121.	13.490	84.692	206486.	71.202
3000.00	14.785	40599.	13.533	85.194	214981.	71.660
3100.00	14.792	42078.	13.574	85.678	223525.	72.105
3200.00	14.799	43557.	13.612	86.148	232116.	72.536
3300.00	14.805	45038.	13.648	86.604	240754.	72.956
3400.00	14.811	46518.	13.682	87.046	249436.	73.364
3500.00	14.816	48000.	13.714	87.475	258162.	73.761
3600.00	14.821	49482.	13.745	87.893	266931.	74.148
3700.00	14.825	50964.	13.774	88.299	275741.	74.525
3800.00	14.829	52446.	13.802	88.694	284590.	74.892
3900.00	14.833	53930.	13.828	89.079	293479.	75.251
4000.00	14.836	55413.	13.853	89.455	302406.	75.602
4100.00	14.839	56897.	13.877	89.821	311370.	75.944
4200.00	14.842	58381.	13.900	90.179	320370.	76.279
4300.00	14.845	59865.	13.922	90.528	329405.	76.606
4400.00	14.848	61350.	13.943	90.870	338475.	76.926
4500.00	14.850	62835.	13.963	91.203	347579.	77.240
4600.00	14.852	64320.	13.983	91.530	356716.	77.547
4700.00	14.855	65805.	14.001	91.849	365885.	77.848
4800.00	14.857	67291.	14.019	92.162	375085.	78.143
4900.00	14.859	68777.	14.036	92.468	384317.	78.432
5000.00	14.860	70263.	14.053	92.768	393574.	78.716
5100.00	14.862	71749.	14.068	93.063	402870.	78.994
5200.00	14.864	73235.	14.084	93.351	412191.	79.268
5300.00	14.865	74721.	14.098	93.634	421540.	79.536
5400.00	14.866	76208.	14.113	93.912	430918.	79.800
5500.00	14.868	77695.	14.126	94.185	440323.	80.059
5600.00	14.869	79182.	14.140	94.453	449755.	80.313
5700.00	14.870	80668.	14.152	94.716	459213.	80.564
5800.00	14.871	82156.	14.165	94.975	468698.	80.810
5900.00	14.872	83643.	14.177	95.229	478208.	81.052
6000.00	14.873	85130.	14.188	95.479	487743.	81.291

TABLE 134

MOLAL THERMODYNAMIC PROPERTIES FOR CARBON DIOXIDE UNINEGATIVE ION (CO_2^-)

IDEAL GAS

GRAM FORMULA WT. = 44.01050 GRAMS

T KELVIN = 273.15 + °C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_p^0 - $\frac{\text{CAL}}{\text{K MOL}}$	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ - $\frac{\text{CAL}}{\text{K MOL}}$	S_T^0 - $\frac{\text{CAL}}{\text{K MOL}}$	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ - $\frac{\text{CAL}}{\text{K MOL}}$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.951	794.89	7.949	48.575	4062.6	40.626
200.00	8.169	1597.2	7.986	54.128	9228.3	46.142
273.15	8.577	2208.7	8.086	56.730	13287.	48.644
298.15	8.746	2425.3	8.134	57.489	14714.	49.354
300.00	8.759	2441.4	8.138	57.543	14821.	49.405
373.15	9.295	3101.5	8.312	59.509	19104.	51.198
400.00	9.497	3353.8	8.384	60.152	20711.	51.778
500.00	10.226	4340.5	8.681	62.161	26840.	53.680
600.00	10.863	5395.8	8.993	64.283	33174.	55.290
700.00	11.389	6509.4	9.299	65.999	39689.	56.700
800.00	11.811	7670.2	9.588	67.548	46368.	57.960
900.00	12.148	8868.8	9.854	68.960	53194.	59.105
1000.00	12.417	10097.	10.098	70.254	60156.	60.156
1100.00	12.632	11350.	10.319	71.448	67242.	61.129
1200.00	12.807	12622.	10.519	72.555	74443.	62.036
1300.00	12.950	13910.	10.701	73.585	81750.	62.885
1400.00	13.068	15211.	10.866	74.550	89194.	63.684
1500.00	13.166	16523.	11.016	75.455	96658.	64.439
1600.00	13.248	17844.	11.153	76.307	104247.	65.154
1700.00	13.318	19172.	11.278	77.113	111918.	65.834
1800.00	13.378	20507.	11.393	77.876	119668.	66.482
1900.00	13.429	21848.	11.499	78.600	127492.	67.101
2000.00	13.473	23193.	11.597	79.290	135387.	67.694
2100.00	13.512	24542.	11.687	79.949	143349.	68.262
2200.00	13.546	25895.	11.771	80.578	151376.	68.807
2300.00	13.575	27251.	11.849	81.181	159464.	69.332
2400.00	13.602	28610.	11.921	81.759	167611.	69.838
2500.00	13.625	29971.	11.989	82.315	175815.	70.326
2600.00	13.646	31335.	12.052	82.850	184073.	70.798
2700.00	13.664	32701.	12.111	83.365	192384.	71.254
2800.00	13.681	34068.	12.167	83.862	200746.	71.695
2900.00	13.696	35437.	12.220	84.343	209156.	72.123
3000.00	13.710	36807.	12.269	84.807	217614.	72.538
3100.00	13.722	38179.	12.316	85.257	226117.	72.941
3200.00	13.734	39551.	12.360	85.693	234664.	73.333
3300.00	13.744	40925.	12.402	86.116	243255.	73.714
3400.00	13.753	42300.	12.441	86.528	251887.	74.085
3500.00	13.762	43676.	12.479	86.929	260560.	74.446
3600.00	13.770	45053.	12.515	87.318	269272.	74.798
3700.00	13.777	46430.	12.549	87.690	278025.	75.141
3800.00	13.784	47808.	12.581	88.057	286809.	75.476
3900.00	13.790	49187.	12.612	88.416	295633.	75.803
4000.00	13.796	50566.	12.642	88.765	304492.	76.123
4100.00	13.802	51946.	12.670	89.106	313386.	76.436
4200.00	13.807	53326.	12.697	89.438	322313.	76.741
4300.00	13.811	54707.	12.723	89.763	331273.	77.040
4400.00	13.816	56089.	12.748	90.081	340265.	77.333
4500.00	13.820	57471.	12.771	90.391	349289.	77.620
4600.00	13.824	58853.	12.794	90.695	358343.	77.901
4700.00	13.827	60235.	12.816	90.992	367428.	78.176
4800.00	13.831	61618.	12.837	91.283	376542.	78.446
4900.00	13.834	63001.	12.858	91.569	385684.	78.711
5000.00	13.837	64385.	12.877	91.848	394855.	78.971
5100.00	13.840	65769.	12.896	92.122	404054.	79.226
5200.00	13.842	67153.	12.914	92.391	413280.	79.477
5300.00	13.845	68537.	12.932	92.655	422532.	79.723
5400.00	13.847	69922.	12.949	92.914	431810.	79.965
5500.00	13.849	71307.	12.965	93.168	441114.	80.203
5600.00	13.852	72692.	12.981	93.417	450444.	80.436
5700.00	13.854	74077.	12.996	93.662	459798.	80.666
5800.00	13.856	75462.	13.011	93.903	469176.	80.892
5900.00	13.857	76848.	13.025	94.140	478578.	81.115
6000.00	13.859	78234.	13.039	94.373	488004.	81.334

TABLE 135

MOLAL THERMODYNAMIC PROPERTIES FOR DIMERIC CARBON UNINEGATIVE ION (C_2^-)

IDEAL GAS

GRAM FORMULA WT. = 24.02285 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T	C_P^0	$(H_T^0 - H_0^0)$	$(H_T^0 - H_0^0)/T$	S_T^0	$-(G_T^0 - H_0^0)$	$-(G_T^0 - H_0^0)/T$
KELVIN	-K CAL MOL	CAL MOL	-K CAL MOL	-K CAL MOL	CAL MOL	-K CAL MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.110	695.98	6.960	39.299	3233.9	32.339
200.00	8.225	1463.8	7.319	44.574	7451.0	37.255
273.15	8.484	2078.4	7.609	47.191	10811.	39.582
298.15	8.472	2290.4	7.682	47.934	12001.	40.252
300.00	8.470	2306.1	7.687	47.986	12089.	40.299
373.15	8.336	2921.1	7.828	49.821	15669.	41.993
400.00	8.282	3144.2	7.861	50.399	17015.	42.538
500.00	8.151	3964.8	7.930	52.230	22150.	44.301
600.00	8.127	4778.0	7.963	53.713	27449.	45.750
700.00	8.170	5592.5	7.989	54.968	32885.	46.979
800.00	8.241	6412.9	8.016	56.064	38438.	48.048
900.00	8.320	7241.0	8.046	57.039	44094.	48.993
1000.00	8.397	8076.9	8.077	57.920	49842.	49.843
1100.00	8.468	8920.3	8.109	58.723	55675.	50.614
1200.00	8.531	9770.3	8.142	59.463	61585.	51.321
1300.00	8.587	10626.	8.174	60.148	67566.	51.974
1400.00	8.636	11487.	8.205	60.786	73613.	52.581
1500.00	8.679	12353.	8.235	61.384	79727.	53.148
1600.00	8.717	13223.	8.264	61.945	85882.	53.681
1700.00	8.751	14096.	8.292	62.475	92110.	54.182
1800.00	8.781	14973.	8.318	62.976	98382.	54.657
1900.00	8.808	15852.	8.343	63.451	104704.	55.108
2000.00	8.832	16734.	8.367	63.903	111072.	55.536
2100.00	8.854	17619.	8.390	64.335	117484.	55.945
2200.00	8.874	18505.	8.412	64.747	123938.	56.336
2300.00	8.892	19393.	8.432	65.142	130433.	56.710
2400.00	8.909	20283.	8.452	65.521	136966.	57.069
2500.00	8.925	21175.	8.470	65.885	143537.	57.415
2600.00	8.939	22068.	8.488	66.235	150143.	57.747
2700.00	8.953	22963.	8.505	66.573	156783.	58.068
2800.00	8.965	23859.	8.521	66.899	163457.	58.378
2900.00	8.977	24756.	8.537	67.214	170163.	58.677
3000.00	8.989	25654.	8.552	67.518	176899.	58.967
3100.00	8.999	26554.	8.566	67.813	183666.	59.247
3200.00	9.009	27454.	8.579	68.099	190462.	59.519
3300.00	9.019	28355.	8.593	68.376	197285.	59.784
3400.00	9.029	29258.	8.605	68.646	204137.	60.040
3500.00	9.038	30161.	8.618	68.907	211014.	60.290
3600.00	9.046	31065.	8.629	69.162	217918.	60.533
3700.00	9.055	31970.	8.641	69.410	224846.	60.769
3800.00	9.063	32876.	8.652	69.652	231800.	61.000
3900.00	9.071	33783.	8.662	69.887	238777.	61.225
4000.00	9.078	34690.	8.673	70.117	245777.	61.444
4100.00	9.086	35599.	8.683	70.341	252800.	61.659
4200.00	9.093	36508.	8.692	70.560	259845.	61.868
4300.00	9.100	37417.	8.702	70.774	266912.	62.073
4400.00	9.107	38328.	8.711	70.984	274000.	62.273
4500.00	9.114	39239.	8.720	71.188	281108.	62.469
4600.00	9.121	40150.	8.728	71.389	288237.	62.660
4700.00	9.127	41063.	8.737	71.585	295386.	62.848
4800.00	9.134	41976.	8.745	71.777	302554.	63.032
4900.00	9.140	42890.	8.753	71.966	309741.	63.213
5000.00	9.147	43804.	8.761	72.150	316947.	63.390
5100.00	9.153	44719.	8.769	72.332	324171.	63.563
5200.00	9.159	45635.	8.776	72.509	331413.	63.733
5300.00	9.165	46551.	8.783	72.684	338673.	63.901
5400.00	9.171	47468.	8.790	72.855	345950.	64.065
5500.00	9.177	48385.	8.797	73.024	353244.	64.226
5600.00	9.183	49303.	8.804	73.189	360555.	64.385
5700.00	9.189	50222.	8.811	73.352	367882.	64.541
5800.00	9.195	51141.	8.817	73.511	375225.	64.694
5900.00	9.200	52060.	8.824	73.669	382584.	64.845
6000.00	9.206	52981.	8.830	73.823	389958.	64.993

TABLE 136

MOLAL THERMODYNAMIC PROPERTIES FOR CCH RADICAL (C_2H)

IDEAL GAS

GRAM FORMULA WT. = 25.03027 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_P^0 --CAL-- K MOL	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ --CAL-- K MOL	S_T^0 --CAL-- K MOL	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ --CAL-- K MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	6.989	694.46	6.945	42.563	3561.8	35.618
200.00	7.816	1426.6	7.133	47.604	8094.3	40.471
273.15	8.627	2028.8	7.427	50.164	11673.	42.736
298.15	8.868	2247.5	7.538	50.930	12937.	43.392
300.00	8.885	2263.9	7.546	50.985	13031.	43.438
373.15	9.472	2936.3	7.869	52.988	16836.	45.119
400.00	9.655	3193.1	7.983	53.652	18267.	45.670
500.00	10.234	4188.6	8.377	55.871	23747.	47.494
600.00	10.716	5236.6	8.728	57.781	29431.	49.053
700.00	11.141	6329.9	9.043	59.465	35295.	50.423
800.00	11.523	7463.4	9.329	60.978	41319.	51.649
900.00	11.868	8633.3	9.593	62.356	47487.	52.763
1000.00	12.178	9835.9	9.836	63.623	53786.	53.787
1100.00	12.457	11067.	10.062	64.797	60208.	54.735
1200.00	12.707	12325.	10.272	65.892	66743.	55.620
1300.00	12.923	13608.	10.468	66.918	73384.	56.450
1400.00	13.135	14912.	10.651	67.884	80125.	57.232
1500.00	13.319	16234.	10.823	68.796	86959.	57.973
1600.00	13.485	17575.	10.985	69.661	93882.	58.677
1700.00	13.636	18931.	11.136	70.483	100890.	59.347
1800.00	13.774	20302.	11.279	71.267	107978.	59.988
1900.00	13.901	21685.	11.414	72.015	115142.	60.601
2000.00	14.016	23081.	11.541	72.731	122380.	61.190
2100.00	14.122	24488.	11.661	73.417	129687.	61.756
2200.00	14.220	25906.	11.775	74.077	137062.	62.301
2300.00	14.310	27332.	11.884	74.711	144502.	62.827
2400.00	14.392	28767.	11.987	75.321	152003.	63.335
2500.00	14.468	30210.	12.084	75.911	159565.	63.826
2600.00	14.537	31661.	12.177	76.479	167185.	64.302
2700.00	14.601	33118.	12.266	77.029	174860.	64.763
2800.00	14.660	34581.	12.350	77.561	182590.	65.211
2900.00	14.714	36049.	12.431	78.077	190372.	65.646
3000.00	14.763	37523.	12.508	78.576	198205.	66.068
3100.00	14.808	39002.	12.581	79.061	206087.	66.480
3200.00	14.849	40485.	12.652	79.532	214017.	66.880
3300.00	14.887	41971.	12.719	79.989	221993.	67.271
3400.00	14.921	43462.	12.783	80.434	230014.	67.651
3500.00	14.952	44956.	12.845	80.867	238079.	68.023
3600.00	14.981	46452.	12.904	81.289	246187.	68.385
3700.00	15.007	47952.	12.960	81.700	254337.	68.740
3800.00	15.030	49454.	13.014	82.100	262527.	69.086
3900.00	15.051	50958.	13.066	82.491	270757.	69.425
4000.00	15.070	52464.	13.116	82.872	279025.	69.756
4100.00	15.088	53972.	13.164	83.245	287331.	70.081
4200.00	15.103	55481.	13.210	83.608	295674.	70.399
4300.00	15.117	56992.	13.254	83.964	304052.	70.710
4400.00	15.129	58505.	13.297	84.312	312466.	71.015
4500.00	15.140	60018.	13.337	84.652	320914.	71.314
4600.00	15.150	61533.	13.377	84.985	329396.	71.608
4700.00	15.159	63048.	13.415	85.311	337911.	71.896
4800.00	15.167	64564.	13.451	85.630	346458.	72.179
4900.00	15.173	66081.	13.486	85.943	355037.	72.457
5000.00	15.179	67599.	13.520	86.249	363646.	72.729
5100.00	15.184	69117.	13.552	86.550	372286.	72.997
5200.00	15.188	70636.	13.584	86.845	380956.	73.261
5300.00	15.192	72155.	13.614	87.134	389655.	73.520
5400.00	15.195	73674.	13.643	87.418	398383.	73.775
5500.00	15.197	75194.	13.672	87.697	407139.	74.025
5600.00	15.199	76714.	13.699	87.971	415922.	74.272
5700.00	15.201	78234.	13.725	88.240	424733.	74.515
5800.00	15.202	79754.	13.751	88.504	433570.	74.754
5900.00	15.202	81274.	13.775	88.764	442433.	74.989
6000.00	15.202	82794.	13.799	89.020	451323.	75.220

TABLE 137

MOLAL THERMODYNAMIC PROPERTIES FOR CNC RADICAL (C₂N)

IDEAL GAS

GRAM FORMULA WT. = 38.02900 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C _P -K CAL MOL	(H _T ⁰ -H ₀ ⁰) CAL MOL	(H _T ⁰ -H ₀ ⁰)/T -K CAL MOL	S _T ⁰ -K CAL MOL	-(G _T ⁰ -H ₀ ⁰) CAL MOL	-(G _T ⁰ -H ₀ ⁰)/T -K CAL MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.878	744.04	7.440	44.959	3751.8	37.518
200.00	9.723	1631.8	8.159	51.038	8575.8	42.879
273.15	10.654	2378.2	8.707	54.211	12429.	45.504
298.15	10.935	2648.1	8.882	55.156	13796.	46.275
300.00	10.955	2668.4	8.895	55.224	13898.	46.330
373.15	11.681	3497.1	9.372	57.693	18031.	48.321
400.00	11.914	3813.9	9.535	58.513	19591.	48.978
500.00	12.630	5043.0	10.086	61.253	25583.	51.167
600.00	13.147	6333.3	10.555	63.604	31828.	53.048
700.00	13.521	7667.7	10.954	65.660	38294.	54.706
800.00	13.794	9034.1	11.293	67.484	44953.	56.191
900.00	13.997	10424.	11.582	69.121	51784.	57.539
1000.00	14.151	11831.	11.832	70.604	58772.	58.772
1100.00	14.270	13253.	12.048	71.959	65901.	59.910
1200.00	14.363	14684.	12.237	73.204	73160.	60.967
1300.00	14.438	16125.	12.404	74.357	80539.	61.953
1400.00	14.499	17572.	12.551	75.429	88029.	62.878
1500.00	14.548	19024.	12.683	76.431	95622.	63.748
1600.00	14.589	20481.	12.801	77.372	103313.	64.571
1700.00	14.624	21942.	12.907	78.257	111095.	65.350
1800.00	14.653	23406.	13.003	79.094	118963.	66.091
1900.00	14.678	24872.	13.091	79.887	126912.	66.796
2000.00	14.699	26341.	13.171	80.640	134939.	67.470
2100.00	14.718	27812.	13.244	81.358	143039.	68.114
2200.00	14.734	29285.	13.311	82.043	151209.	68.732
2300.00	14.748	30759.	13.374	82.698	159447.	69.325
2400.00	14.761	32234.	13.431	83.326	167748.	69.895
2500.00	14.772	33711.	13.484	83.929	176111.	70.445
2600.00	14.781	35188.	13.534	84.509	184533.	70.974
2700.00	14.790	36667.	13.581	85.067	193012.	71.486
2800.00	14.798	38146.	13.624	85.605	201546.	71.981
2900.00	14.805	39627.	13.664	86.124	210132.	72.460
3000.00	14.812	41107.	13.703	86.626	218770.	72.923
3100.00	14.818	42589.	13.738	87.112	227457.	73.373
3200.00	14.823	44071.	13.772	87.582	236192.	73.810
3300.00	14.828	45553.	13.804	88.039	244973.	74.234
3400.00	14.833	47036.	13.834	88.481	253799.	74.647
3500.00	14.837	48520.	13.863	88.911	262669.	75.048
3600.00	14.841	50004.	13.890	89.329	271581.	75.439
3700.00	14.845	51488.	13.916	89.736	280534.	75.820
3800.00	14.849	52973.	13.940	90.132	289528.	76.192
3900.00	14.853	54458.	13.964	90.518	298560.	76.554
4000.00	14.856	55943.	13.986	90.894	307631.	76.908
4100.00	14.860	57429.	14.007	91.261	316739.	77.254
4200.00	14.864	58915.	14.028	91.619	325883.	77.591
4300.00	14.868	60402.	14.047	91.969	335062.	77.922
4400.00	14.872	61889.	14.066	92.311	344276.	78.245
4500.00	14.876	63376.	14.084	92.645	353524.	78.561
4600.00	14.880	64864.	14.101	92.972	362805.	78.871
4700.00	14.884	66352.	14.118	93.292	372118.	79.174
4800.00	14.889	67841.	14.134	93.605	381463.	79.472
4900.00	14.894	69330.	14.149	93.912	390839.	79.763
5000.00	14.899	70820.	14.164	94.213	400246.	80.049
5100.00	14.905	72310.	14.179	94.508	409682.	80.330
5200.00	14.911	73801.	14.193	94.798	419147.	80.605
5300.00	14.917	75292.	14.206	95.082	428641.	80.876
5400.00	14.923	76784.	14.219	95.361	438163.	81.141
5500.00	14.930	78277.	14.232	95.635	447713.	81.402
5600.00	14.937	79770.	14.245	95.904	457290.	81.659
5700.00	14.945	81264.	14.257	96.168	466894.	81.911
5800.00	14.953	82759.	14.269	96.428	476523.	82.159
5900.00	14.961	84255.	14.281	96.684	486179.	82.403
6000.00	14.970	85751.	14.292	96.935	495860.	82.643

TABLE 138

MOLAL THERMODYNAMIC PROPERTIES FOR CCO RADICAL (C₂O)

IDEAL GAS

GRAM FORMULA WT.= 40.02170 GRAMS

T KELVIN=273.15+T DEG C

1 CAL=4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C _P ⁰ -CAL- -K MOL-	(H _T ⁰ -H ₀ ⁰) CAL MOL	(H _T ⁰ -H ₀ ⁰)/T -CAL- -K MOL-	S _T ⁰ -CAL- -K MOL-	-(G _T ⁰ -H ₀ ⁰) CAL MOL	-(G _T ⁰ -H ₀ ⁰)/T -CAL- -K MOL-
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	7.456	704.22	7.042	46.045	3900.3	39.003
200.00	9.209	1542.2	7.711	51.782	8814.2	44.071
273.15	10.057	2248.6	8.232	54.785	12716.	46.553
298.15	10.292	2503.0	8.395	55.676	14096.	47.281
300.00	10.309	2522.1	8.407	55.740	14200.	47.333
373.15	10.902	3298.6	8.840	58.054	18364.	49.214
400.00	11.094	3593.9	8.985	58.818	19933.	49.833
500.00	11.722	4735.7	9.471	61.363	25946.	51.892
600.00	12.243	5934.7	9.891	63.548	32194.	53.657
700.00	12.682	7181.6	10.259	65.469	38646.	55.210
800.00	13.056	8469.0	10.586	67.188	45281.	56.601
900.00	13.377	9791.0	10.879	68.744	52079.	57.866
1000.00	13.657	11143.	11.143	70.169	59025.	59.026
1100.00	13.903	12521.	11.383	71.482	66109.	60.099
1200.00	14.122	13922.	11.602	72.701	73318.	61.099
1300.00	14.315	15344.	11.804	73.840	80646.	62.036
1400.00	14.488	16785.	11.989	74.907	88084.	62.917
1500.00	14.641	18241.	12.161	75.912	95625.	63.751
1600.00	14.776	19712.	12.320	76.861	103265.	64.541
1700.00	14.896	21196.	12.468	77.760	110996.	65.292
1800.00	15.001	22691.	12.606	78.615	118815.	66.009
1900.00	15.092	24196.	12.735	79.429	126718.	66.694
2000.00	15.172	25709.	12.855	80.205	134700.	67.350
2100.00	15.241	27230.	12.967	80.947	142757.	67.980
2200.00	15.300	28757.	13.072	81.657	150888.	68.586
2300.00	15.350	30289.	13.170	82.338	159088.	69.169
2400.00	15.392	31827.	13.261	82.993	167355.	69.731
2500.00	15.428	33368.	13.347	83.622	175686.	70.274
2600.00	15.457	34912.	13.428	84.227	184078.	70.799
2700.00	15.480	36459.	13.503	84.811	192530.	71.308
2800.00	15.499	38008.	13.574	85.374	201040.	71.800
2900.00	15.513	39558.	13.641	85.919	209605.	72.278
3000.00	15.524	41110.	13.704	86.445	218223.	72.741
3100.00	15.531	42663.	13.762	86.954	226893.	73.191
3200.00	15.536	44216.	13.818	87.447	235613.	73.629
3300.00	15.538	45770.	13.870	87.925	244382.	74.055
3400.00	15.538	47324.	13.919	88.389	253198.	74.470
3500.00	15.536	48878.	13.965	88.839	262059.	74.874
3600.00	15.533	50431.	14.009	89.277	270965.	75.268
3700.00	15.528	51984.	14.050	89.702	279914.	75.653
3800.00	15.523	53537.	14.089	90.117	288905.	76.028
3900.00	15.516	55089.	14.125	90.520	297937.	76.394
4000.00	15.509	56640.	14.160	90.912	307009.	76.752
4100.00	15.501	58190.	14.193	91.295	316119.	77.102
4200.00	15.492	59740.	14.224	91.669	325267.	77.445
4300.00	15.483	61289.	14.253	92.033	334453.	77.780
4400.00	15.474	62837.	14.281	92.389	343674.	78.108
4500.00	15.465	64384.	14.308	92.737	352930.	78.429
4600.00	15.455	65930.	14.333	93.076	362221.	78.744
4700.00	15.445	67475.	14.356	93.409	371545.	79.052
4800.00	15.435	69019.	14.379	93.734	380902.	79.355
4900.00	15.426	70562.	14.400	94.052	390292.	79.651
5000.00	15.416	72104.	14.421	94.363	399713.	79.943
5100.00	15.406	73645.	14.440	94.669	409164.	80.228
5200.00	15.396	75185.	14.459	94.968	418646.	80.509
5300.00	15.386	76724.	14.476	95.261	428158.	80.785
5400.00	15.377	78262.	14.493	95.548	437698.	81.055
5500.00	15.368	79800.	14.509	95.830	447267.	81.321
5600.00	15.358	81336.	14.524	96.107	456864.	81.583
5700.00	15.349	82871.	14.539	96.379	466488.	81.840
5800.00	15.340	84406.	14.553	96.646	476140.	82.093
5900.00	15.331	85939.	14.566	96.908	485817.	82.342
6000.00	15.323	87472.	14.579	97.166	495521.	82.587

TABLE 139

MOLAL THERMODYNAMIC PROPERTIES FOR PROTON (H⁺)

IDEAL GAS

GRAM FORMULA WT.= 1.00742 GRAMS

T KELVIN=273.15+T DEG C

1 CAL=4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C _p ⁰ - $\frac{\text{CAL}}{\text{K MOL}}$	(H _T ⁰ -H ₀ ⁰) CAL MOL	(H _T ⁰ -H ₀ ⁰)/T - $\frac{\text{CAL}}{\text{K MOL}}$	S _T ⁰ - $\frac{\text{CAL}}{\text{K MOL}}$	-(G _T ⁰ -H ₀ ⁰) CAL MOL	-(G _T ⁰ -H ₀ ⁰)/T - $\frac{\text{CAL}}{\text{K MOL}}$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	4.968	496.79	4.968	20.584	1561.7	15.617
200.00	4.968	993.58	4.968	24.028	3812.0	19.060
273.15	4.968	1357.0	4.968	25.576	5629.2	20.609
298.15	4.968	1481.2	4.968	26.012	6274.2	21.044
300.00	4.968	1490.4	4.968	26.042	6322.3	21.074
373.15	4.968	1853.8	4.968	27.126	8268.4	22.158
400.00	4.968	1987.2	4.968	27.471	9001.4	22.504
500.00	4.968	2483.9	4.968	28.580	11806.	23.612
600.00	4.968	2980.7	4.968	29.486	14710.	24.518
700.00	4.968	3477.5	4.968	30.252	17698.	25.284
800.00	4.968	3974.3	4.968	30.915	20757.	25.947
900.00	4.968	4471.1	4.968	31.500	23879.	26.532
1000.00	4.968	4967.9	4.968	32.023	27055.	27.056
1100.00	4.968	5464.7	4.968	32.497	30282.	27.529
1200.00	4.968	5961.5	4.968	32.929	33553.	27.961
1300.00	4.968	6458.3	4.968	33.327	36866.	28.359
1400.00	4.968	6955.1	4.968	33.695	40218.	28.727
1500.00	4.968	7451.8	4.968	34.038	43604.	29.070
1600.00	4.968	7948.6	4.968	34.358	47024.	29.391
1700.00	4.968	8445.4	4.968	34.660	50475.	29.692
1800.00	4.968	8942.2	4.968	34.944	53956.	29.976
1900.00	4.968	9439.0	4.968	35.212	57464.	30.244
2000.00	4.968	9935.8	4.968	35.467	60998.	30.499
2100.00	4.968	10432.	4.968	35.709	64557.	30.741
2200.00	4.968	10929.	4.968	35.940	68139.	30.973
2300.00	4.968	11426.	4.968	36.161	71744.	31.193
2400.00	4.968	11923.	4.968	36.373	75371.	31.405
2500.00	4.968	12419.	4.968	36.576	79019.	31.608
2600.00	4.968	12916.	4.968	36.770	82686.	31.802
2700.00	4.968	13413.	4.968	36.958	86372.	31.990
2800.00	4.968	13910.	4.968	37.139	90077.	32.171
2900.00	4.968	14406.	4.968	37.313	93800.	32.345
3000.00	4.968	14903.	4.968	37.481	97540.	32.513
3100.00	4.968	15400.	4.968	37.644	101296.	32.676
3200.00	4.968	15897.	4.968	37.802	105068.	32.834
3300.00	4.968	16394.	4.968	37.955	108856.	32.987
3400.00	4.968	16890.	4.968	38.103	112659.	33.135
3500.00	4.968	17387.	4.968	38.247	116477.	33.279
3600.00	4.968	17884.	4.968	38.387	120308.	33.419
3700.00	4.968	18381.	4.968	38.523	124154.	33.555
3800.00	4.968	18878.	4.968	38.656	128013.	33.688
3900.00	4.968	19374.	4.968	38.785	131885.	33.817
4000.00	4.968	19871.	4.968	38.910	135770.	33.943
4100.00	4.968	20368.	4.968	39.033	139667.	34.065
4200.00	4.968	20865.	4.968	39.153	143576.	34.185
4300.00	4.968	21362.	4.968	39.270	147497.	34.302
4400.00	4.968	21858.	4.968	39.384	151430.	34.416
4500.00	4.968	22355.	4.968	39.496	155374.	34.528
4600.00	4.968	22852.	4.968	39.605	159329.	34.637
4700.00	4.968	23349.	4.968	39.712	163295.	34.744
4800.00	4.968	23845.	4.968	39.816	167271.	34.848
4900.00	4.968	24342.	4.968	39.919	171258.	34.951
5000.00	4.968	24839.	4.968	40.019	175255.	35.051
5100.00	4.968	25336.	4.968	40.117	179262.	35.149
5200.00	4.968	25833.	4.968	40.214	183279.	35.246
5300.00	4.968	26329.	4.968	40.308	187305.	35.341
5400.00	4.968	26826.	4.968	40.401	191340.	35.433
5500.00	4.968	27323.	4.968	40.493	195385.	35.525
5600.00	4.968	27820.	4.968	40.582	199439.	35.614
5700.00	4.968	28317.	4.968	40.670	203501.	35.702
5800.00	4.968	28813.	4.968	40.756	207573.	35.788
5900.00	4.968	29310.	4.968	40.841	211652.	35.873
6000.00	4.968	29807.	4.968	40.925	215741.	35.957

TABLE 140

MOLAL THERMODYNAMIC PROPERTIES FOR NITRIC OXIDE UNIPOSITIVE ION (NO^+)
IDEAL GAS

GRAM FORMULA WT. = 30.00555 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_p^0 --K CAL-- MOL	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ --K CAL-- MOL	S_T^0 --K CAL-- MOL	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ --K CAL-- MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	6.956	693.64	6.936	39.748	3281.2	32.812
200.00	6.957	1389.3	6.946	44.570	7524.7	37.623
273.15	6.959	1898.2	6.949	46.738	10868.	39.789
298.15	6.961	2072.2	6.950	47.348	12044.	40.398
300.00	6.961	2085.1	6.950	47.391	12132.	40.441
373.15	6.977	2594.7	6.954	48.911	15656.	41.957
400.00	6.989	2782.2	6.956	49.396	16976.	42.441
500.00	7.067	3484.6	6.969	50.963	21997.	43.994
600.00	7.191	4197.2	6.995	52.262	27160.	45.267
700.00	7.344	4923.8	7.034	53.382	32443.	46.348
800.00	7.505	5666.2	7.083	54.373	37832.	47.290
900.00	7.662	6424.7	7.139	55.266	43314.	48.128
1000.00	7.807	7198.3	7.198	56.081	48882.	48.883
1100.00	7.938	7985.7	7.260	56.831	54528.	49.572
1200.00	8.054	8785.4	7.321	57.527	60247.	50.206
1300.00	8.156	9595.9	7.381	58.176	66032.	50.794
1400.00	8.245	10416.	7.440	58.784	71881.	51.344
1500.00	8.323	11244.	7.496	59.355	77788.	51.859
1600.00	8.392	12080.	7.550	59.895	83751.	52.344
1700.00	8.452	12922.	7.602	60.405	89766.	52.804
1800.00	8.506	13770.	7.650	60.890	95831.	53.240
1900.00	8.553	14623.	7.697	61.351	101943.	53.654
2000.00	8.595	15481.	7.741	61.791	108100.	54.050
2100.00	8.633	16342.	7.782	62.211	114300.	54.429
2200.00	8.667	17207.	7.822	62.614	120542.	54.792
2300.00	8.697	18075.	7.859	62.999	126823.	55.140
2400.00	8.725	18946.	7.895	63.370	133141.	55.476
2500.00	8.750	19820.	7.928	63.727	139496.	55.799
2600.00	8.774	20696.	7.960	64.071	145886.	56.110
2700.00	8.795	21575.	7.991	64.402	152310.	56.411
2800.00	8.814	22455.	8.020	64.722	158766.	56.702
2900.00	8.832	23338.	8.048	65.032	165254.	56.984
3000.00	8.849	24222.	8.074	65.332	171772.	57.258
3100.00	8.865	25107.	8.099	65.622	178320.	57.523
3200.00	8.879	25995.	8.123	65.904	184896.	57.780
3300.00	8.893	26883.	8.147	66.177	191500.	58.031
3400.00	8.906	27773.	8.169	66.443	198132.	58.274
3500.00	8.918	28664.	8.190	66.701	204789.	58.511
3600.00	8.929	29557.	8.210	66.953	211472.	58.742
3700.00	8.940	30450.	8.230	67.197	218179.	58.967
3800.00	8.951	31345.	8.249	67.436	224911.	59.187
3900.00	8.961	32240.	8.267	67.669	231666.	59.402
4000.00	8.970	33137.	8.284	67.896	238444.	59.611
4100.00	8.979	34034.	8.301	68.117	245245.	59.816
4200.00	8.988	34933.	8.317	68.334	252068.	60.016
4300.00	8.996	35832.	8.333	68.545	258912.	60.212
4400.00	9.004	36732.	8.348	68.752	265776.	60.404
4500.00	9.012	37633.	8.363	68.955	272662.	60.592
4600.00	9.019	38534.	8.377	69.153	279567.	60.776
4700.00	9.026	39436.	8.391	69.347	286492.	60.956
4800.00	9.033	40339.	8.404	69.537	293436.	61.133
4900.00	9.040	41243.	8.417	69.723	300399.	61.306
5000.00	9.047	42148.	8.430	69.906	307381.	61.476
5100.00	9.053	43053.	8.442	70.085	314381.	61.643
5200.00	9.060	43958.	8.454	70.261	321398.	61.807
5300.00	9.066	44864.	8.465	70.434	328433.	61.969
5400.00	9.072	45771.	8.476	70.603	335484.	62.127
5500.00	9.078	46679.	8.487	70.770	342553.	62.282
5600.00	9.084	47587.	8.498	70.933	349633.	62.435
5700.00	9.089	48496.	8.508	71.094	356740.	62.586
5800.00	9.095	49405.	8.518	71.252	363857.	62.734
5900.00	9.100	50314.	8.528	71.408	370990.	62.880
6000.00	9.106	51225.	8.538	71.561	378138.	63.023

TABLE 141

MOLAL THERMODYNAMIC PROPERTIES FOR PHOSPHORUS NITRIDE (NP)

IDEAL GAS

GRAM FORMULA WT. = 44.98050 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_p^0 --CAL-- K MOL--	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ --CAL-- K MOL--	S_T^0 --CAL-- K MOL--	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ --CAL-- K MOL--
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	6.956	694.81	6.948	42.809	3586.1	35.861
200.00	6.970	1390.7	6.954	47.633	8135.8	40.679
273.15	7.049	1903.0	6.967	49.815	11703.	42.848
298.15	7.096	2079.8	6.976	50.434	12957.	43.458
300.00	7.100	2092.9	6.976	50.478	13050.	43.502
373.15	7.280	2618.6	7.017	52.045	16802.	45.028
400.00	7.355	2815.0	7.038	52.554	18206.	45.516
500.00	7.636	3564.7	7.129	54.225	23547.	47.096
600.00	7.885	4341.0	7.235	55.640	29043.	48.405
700.00	8.087	5140.0	7.343	56.871	34669.	49.528
800.00	8.248	5957.1	7.446	57.962	40412.	50.516
900.00	8.375	6788.5	7.543	58.941	46258.	51.398
1000.00	8.476	7631.3	7.631	59.829	52197.	52.198
1100.00	8.557	8483.1	7.712	60.641	58221.	52.929
1200.00	8.623	9342.2	7.785	61.388	64323.	53.603
1300.00	8.677	10207.	7.852	62.081	70497.	54.229
1400.00	8.723	11077.	7.912	62.726	76738.	54.813
1500.00	8.761	11951.	7.968	63.329	83041.	55.361
1600.00	8.794	12829.	8.018	63.895	89402.	55.877
1700.00	8.822	13710.	8.065	64.429	95819.	56.364
1800.00	8.847	14593.	8.108	64.934	102287.	56.827
1900.00	8.869	15479.	8.147	65.413	108805.	57.266
2000.00	8.889	16367.	8.184	65.869	115369.	57.685
2100.00	8.907	17257.	8.218	66.303	121978.	58.085
2200.00	8.923	18148.	8.249	66.717	128629.	58.468
2300.00	8.937	19041.	8.279	67.114	135321.	58.835
2400.00	8.951	19936.	8.307	67.495	142051.	59.188
2500.00	8.963	20832.	8.333	67.861	148819.	59.528
2600.00	8.975	21728.	8.357	68.212	155623.	59.855
2700.00	8.986	22627.	8.380	68.551	162461.	60.171
2800.00	8.996	23526.	8.402	68.878	169333.	60.476
2900.00	9.006	24426.	8.423	69.194	176237.	60.771
3000.00	9.015	25327.	8.442	69.500	183171.	61.057
3100.00	9.024	26229.	8.461	69.795	190136.	61.334
3200.00	9.032	27131.	8.479	70.082	197130.	61.603
3300.00	9.040	28035.	8.496	70.360	204152.	61.865
3400.00	9.048	28939.	8.512	70.630	211202.	62.118
3500.00	9.055	29845.	8.527	70.892	218278.	62.365
3600.00	9.063	30751.	8.542	71.148	225380.	62.606
3700.00	9.070	31657.	8.556	71.396	232507.	62.840
3800.00	9.077	32565.	8.570	71.638	239659.	63.068
3900.00	9.084	33473.	8.583	71.874	246835.	63.291
4000.00	9.090	34381.	8.595	72.104	254034.	63.509
4100.00	9.097	35291.	8.608	72.329	261256.	63.722
4200.00	9.103	36200.	8.619	72.548	268499.	63.929
4300.00	9.109	37111.	8.631	72.762	275765.	64.131
4400.00	9.115	38022.	8.642	72.972	283052.	64.330
4500.00	9.121	38934.	8.652	73.176	290359.	64.524
4600.00	9.127	39847.	8.662	73.377	297687.	64.715
4700.00	9.133	40760.	8.672	73.573	305034.	64.901
4800.00	9.139	41673.	8.682	73.766	312401.	65.084
4900.00	9.144	42587.	8.691	73.954	319787.	65.263
5000.00	9.150	43502.	8.700	74.139	327192.	65.438
5100.00	9.156	44417.	8.709	74.320	334615.	65.611
5200.00	9.161	45333.	8.718	74.498	342056.	65.780
5300.00	9.167	46249.	8.726	74.673	349515.	65.946
5400.00	9.172	47166.	8.735	74.844	356990.	66.109
5500.00	9.177	48084.	8.743	75.012	364483.	66.270
5600.00	9.183	49002.	8.750	75.178	371993.	66.427
5700.00	9.188	49920.	8.758	75.340	379519.	66.582
5800.00	9.193	50840.	8.766	75.500	387061.	66.735
5900.00	9.199	51759.	8.773	75.657	394619.	66.885
6000.00	9.204	52679.	8.780	75.812	402192.	67.032

TABLE 142

MOLAL THERMODYNAMIC PROPERTIES FOR DIATOMIC OXYGEN UNINEGATIVE ION (O_2^-)

IDEAL GAS

GRAM FORMULA WT. = 31.99935 GRAMS

T KELVIN = 273.15 + T DEG C

1 CAL = 4.1840 JOULES

STANDARD THERMODYNAMIC FUNCTIONS

T KELVIN	C_p^0 --K CAL-- MOL	$(H_T^0 - H_0^0)$ CAL MOL	$(H_T^0 - H_0^0)/T$ --K CAL-- MOL	S_T^0 --K CAL-- MOL	$-(G_T^0 - H_0^0)$ CAL MOL	$-(G_T^0 - H_0^0)/T$ --K CAL-- MOL
0.00	0.000	0.000	0.000	0.000	0.000	0.000
100.00	6.957	694.42	6.944	42.259	3531.5	35.315
200.00	6.994	1391.1	6.955	47.087	8026.3	40.132
273.15	7.132	1907.0	6.982	49.285	11555.	42.303
298.15	7.202	2086.2	6.997	49.912	12795.	42.915
300.00	7.207	2099.5	6.998	49.957	12837.	42.958
373.15	7.441	2635.1	7.062	51.553	16602.	44.462
400.00	7.529	2836.1	7.090	52.073	17993.	44.983
500.00	7.833	3604.6	7.209	53.787	23288.	46.578
600.00	8.079	4400.6	7.334	55.238	28742.	47.903
700.00	8.268	5218.4	7.455	56.498	34330.	49.043
800.00	8.414	6052.8	7.566	57.612	40036.	50.046
900.00	8.526	6900.0	7.667	58.610	45848.	50.943
1000.00	8.615	7757.3	7.757	59.513	51755.	51.755
1100.00	8.686	8622.4	7.839	60.337	57748.	52.499
1200.00	8.744	9494.0	7.912	61.096	63820.	53.184
1300.00	8.792	10370.	7.978	61.797	69965.	53.820
1400.00	8.832	11252.	8.037	62.450	76178.	54.413
1500.00	8.867	12137.	8.091	63.061	82454.	54.970
1600.00	8.898	13025.	8.141	63.634	88789.	55.493
1700.00	8.924	13916.	8.186	64.174	95180.	55.988
1800.00	8.948	14810.	8.228	64.685	101623.	56.457
1900.00	8.970	15706.	8.266	65.170	108116.	56.903
2000.00	8.990	16604.	8.302	65.630	114656.	57.328
2100.00	9.008	17503.	8.335	66.069	121241.	57.734
2200.00	9.025	18405.	8.366	66.489	127869.	58.123
2300.00	9.041	19308.	8.395	66.890	134538.	58.495
2400.00	9.055	20213.	8.422	67.275	141247.	58.853
2500.00	9.070	21119.	8.448	67.645	147993.	59.197
2600.00	9.083	22027.	8.472	68.001	154775.	59.529
2700.00	9.096	22936.	8.495	68.344	161593.	59.849
2800.00	9.108	23846.	8.517	68.675	168444.	60.159
2900.00	9.120	24758.	8.537	68.995	175328.	60.458
3000.00	9.132	25670.	8.557	69.305	182243.	60.748
3100.00	9.143	26584.	8.576	69.604	189188.	61.029
3200.00	9.154	27499.	8.594	69.895	196162.	61.301
3300.00	9.165	28415.	8.611	70.177	203167.	61.566
3400.00	9.176	29332.	8.627	70.450	210198.	61.823
3500.00	9.187	30250.	8.643	70.716	217257.	62.073
3600.00	9.197	31169.	8.658	70.975	224341.	62.317
3700.00	9.208	32090.	8.673	71.228	231451.	62.555
3800.00	9.219	33011.	8.687	71.473	238587.	62.786
3900.00	9.229	33933.	8.701	71.713	245746.	63.012
4000.00	9.240	34857.	8.714	71.947	252929.	63.232
4100.00	9.250	35781.	8.727	72.175	260135.	63.448
4200.00	9.261	36707.	8.740	72.398	267364.	63.658
4300.00	9.272	37634.	8.752	72.616	274614.	63.864
4400.00	9.283	38561.	8.764	72.829	281887.	64.065
4500.00	9.295	39490.	8.776	73.038	289180.	64.262
4600.00	9.306	40420.	8.787	73.242	296494.	64.455
4700.00	9.318	41352.	8.798	73.443	303829.	64.644
4800.00	9.330	42284.	8.809	73.639	311183.	64.830
4900.00	9.342	43218.	8.820	73.832	318556.	65.012
5000.00	9.355	44152.	8.831	74.020	325949.	65.190
5100.00	9.368	45088.	8.841	74.206	333360.	65.365
5200.00	9.381	46026.	8.851	74.388	340790.	65.537
5300.00	9.394	46965.	8.861	74.567	348238.	65.705
5400.00	9.408	47905.	8.871	74.742	355703.	65.871
5500.00	9.422	48846.	8.881	74.915	363186.	66.034
5600.00	9.436	49789.	8.891	75.085	370686.	66.194
5700.00	9.450	50733.	8.901	75.252	378203.	66.351
5800.00	9.465	51679.	8.910	75.417	385736.	66.506
5900.00	9.481	52626.	8.920	75.579	393286.	66.659
6000.00	9.496	53575.	8.929	75.738	400852.	66.809

Section II.

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

Eugene S. Domalski

Preliminary List of Organic Compounds Proposed for
Listing with Measured Heats of Combustion and Formation
for the Handbook of Thermodynamic Data on Biological Compounds

Organic compounds treated in NBS Reports 8641, 8906, and
9374 constitute the first 71 compounds.

1. L - alanine
2. DL - alanine
3. α - aminobutyric acid
4. γ - aminobutyric acid
5. L - arginine
6. L - asparagine
7. L - asparagine hydrate
8. L - aspartic acid
9. L - cysteine
10. L - cystine
11. L - glutamic acid
12. L - glutamine
13. glycine
14. hippuric acid
15. L - histidine
16. L - hydroxy glutamic acid
17. L - hydroxy proline
18. DL - isoleucine
19. L - isoleucine
20. L - isoserine
21. D - leucine
22. L - leucine
23. DL - leucine

- 24. DL - lysine
- 25. L - methionine
- 26. norleucine
- 27. DL - ornithine
- 28, 29. DL - and L - phenylalanine
- 30. L - proline
- 31. sarcosine
- 32. serine
- 33, 34. DL - and L - threonine
- 35. L - tryptophane
- 36. L - tyrosine
- 37, 38. DL - and L - valine
- 39. adenine
- 40. creatine
- 41. creatine hydrate
- 42. creatinine
- 43. fumaric acid
- 44. α - D - glucose
- 45. α - D - glucose hydrate
- 46. β - D - glucose
- 47. guanine
- 48. hypoxanthine
- 49. maleic acid
- 50. nicotine
- 51. 8 - oxypurine
- 52. pyruvic acid
- 53. D - ribose
- 54. thymine
- 55. uric acid
- 56. xanthine
- 57. alanyl phenylalanine

- 58. alanyl phenylalanine
- 59. glycyl glycine
- 60. glycyl phenylalanine
- 61. glycyl valine
- 62. hippuryl glycine
- 63. leucyl glycine
- 64. seryl serine
- 65. valyl phenylalanine
- 66. glycyl alanyl phenylalanine
- 67. leucyl glycyl glycine
- 68. benzene
- 69. naphthalene
- 70. anthracene
- 71. phenanthrene

Additional amino-acid-related compounds

- 72. glycyl glycine carboxylic acid
- 73. diglycyl glycine
- 74. seryl seryl anhydride
- 75. alanine anhydride
- 76. triglycolamidic acid
- 77. glycyl glycine ethylester
- 78. glycyl valyl anhydride
- 79. formyl - (DL) - leucine
- 80. valyl alanyl anhydride
- 81. tri-glycyl glycine
- 82. α - carbethoxy glycyl glycine ethyl ester
- 83. β - carbethoxy glycyl glycine ethyl ester
- 84. valyl leucyl anhydride
- 85. leucine imide
- 86. phenylalanyl anhydride

87. phenyl glycocoll
88. phenaceturic acid
89. benzoyl alanine
90. p - toluyyl glycine
91. m - toluyyl glycine
92. o - toluyyl glycine
93. anisoyl glycine
94. benzoyl glycine
95. phenylalanine - N - carboxylic acid anhydride
96. glycyl - phenylalanine peptide
97. o - toluyyl alanine
98. p - toluyyl alanine
99. glycyl phenylalanine anhydride
100. glycyl tyrosyl anhydride
101. alanyl phenylalanine anhydride
102. alanyl phenylalanine peptide
103. DL - phenylalanine - N - carboxylic acid dimethyl ester
104. valyl phenylalanine
105. glycyl alanyl phenylalanine
106. valyl phenylalanyl anhydride
107. benzal hippuric azlactone
108. benzal hippuric acid
109. benzoyl phenylalanine
110. ethyl - β - anilino - β - phenyl propionate
111. ethylenediaminetetraacetic acid
112. cholesterol
113. cholesteryl methyl ether
114. phenylalanine polypeptide (benzene soluble)
115. phenylalanine polypeptide (benzene insoluble)
116. sarcosine polypeptide

Polynuclear aromatic compounds

- 117. pyrene
- 118. triphenylene
- 119. chrysene
- 120. 3,4 - benzphenanthrene
- 121. 1,2 - benzanthracene
- 122. tetracene
- 123. perylene
- 124. 9,10 - diphenylanthracene

Aliphatic Alcohols

- 125. methyl alcohol
- 126. ethyl alcohol
- 127. n - propyl alcohol
- 128. n - butyl alcohol
- 129. n - amyl alcohol
- 130. n - hexyl alcohol
- 131. benzyl alcohol

Di - and Poly - Ols

- 132. ethylene glycol
- 133. glycerol
- 134. erythritol
- 135. pentaerythritol
- 136. L - arabitol
- 137. dulcitol
- 138. mannitol
- 139. D - perseitol
- 140. D - gluco - α - heptite
- 141. dipentaerythritol

Phenols

- 142. phenol
- 143. pyrocatechol
- 144. resorcinol
- 145. hydroquinone
- 146. phloroglucinol
- 147. pyrogallol
- 148. o - cresol
- 149. m - cresol
- 150. p - cresol
- 151. orcinol
- 152. α - naphthol
- 153. β - naphthol

Aldehydes

- 154. formaldehyde
- 155. acetaldehyde
- 156. propionaldehyde
- 157. butyraldehyde
- 158. acrolein
- 159. aldol
- 160. valeraldehyde
- 161. α - amino - valeraldehyde
- 162. benzaldehyde
- 163. vanillin
- 164. salicylaldehyde

Ketones

- 165. acetone
- 166. methyl ethyl ketone

- 167. diethyl ketone
- 168. di - n - propyl ketone
- 169. acetophenone
- 170. benzophenone
- 171. formic acid
- 172. acetic acid
- 173. propionic acid
- 174. butyric acid

n - Aliphatic acids

- 175. valeric acid
- 176. caproic acid
- 177. caprylic acid
- 178. pelargonic acid
- 179. capric acid
- 180. undecylic acid
- 181. lauric acid
- 182. myristic acid
- 183. palmitic acid
- 184. stearic acid
- 185. arachic acid
- 186. behenic acid

Hydroxy aliphatic acids

- 187. glyoxylic acid
- 188. glycolic acid
- 189. D - and DL - lactic acid
- 190. mesoxalic acid
- 191. DL - β - hydroxybutyric acid
- 192. hydroxyisobutyric acid

- 193. levulinic acid
- 194. dihydroxybehenic acid
- 195. D - gluconic acid
- 196. D - galactic acid
- 197. D - mannonic acid
- 198. L - ascorbic acid

Unsaturated aliphatic acids

- 199. acrylic acid
- 200. crotonic acid
- 201. tiglic acid
- 202. angelic acid
- 203. sorbic acid
- 204. hydrosorbic acid
- 205. undecylenic acid
- 206. elaidic acid
- 207. oleic acid
- 208. brassidic acid
- 209. erucic acid

Dicarboxylic acids

- 210. oxalic acid
- 211. malonic acid
- 212. succinic acid
- 213. glutaric acid
- 214. adipic acid

Hydroxy dicarboxylic acids

- 215. tartaric acid (racemic)
- 216. tartaric acid (meso)
- 217. D - tartaric acid
- 218. tartaric acid (racemic, hydrate)
- 219. DL - trihydroxyglutaric acid
- 220. citric acid (anhydrous)
- 221. citric acid (monohydrate)
- 222. allomucic acid
- 223. mucic acid
- 224. citraconic acid
- 225. itaconic acid
- 226. mesaconic acid
- 227. α - β - hydromucic acid
- 228. β - γ - hydromucic acid
- 229. aconitric acid
- 230. tetraconic acid

Aromatic acids

- 231. benzoic acid
- 232. salicylic acid
- 233. o - phthalic acid
- 234. m - phthalic acid
- 235. p - phthalic acid

Phenylated aliphatic acids

- 236. phenyl acetic acid
- 237. mandelic acid
- 238. phenyl glyoxylic acid

- 239. phenoxyacetic acid
- 240. phenyl glyceric acid
- 241. atropic acid
- 242. cinnamic acid (cis)
- 243. cinnamic acid (trans)
- 244. cholic acid

Acid Anhydrides

- 245. acetic anhydride
- 246. maleic anhydride
- 247. fumaric anhydride

Monosaccharides

- 248. α - D - xylose
- 249. D - arabinose
- 250. β - L - arabinose
- 251. α - D - galactose
- 252. D - mannose
- 253. D - fucose
- 254. L - sorbose
- 255. β - L - rhamnose
- 256. α - L - rhamnose monohydrate
- 257. β - D - fructose
- 258. levo - glucosan
- 259. α - methyl - D - glucopyranoside
- 260. β - methyl - D - glucopyranoside
- 261. β - methyl - D - glucofuranoside
- 262. α - gluco - α - heptose
- 263. levo - glucosan triacetate

- 264. 1,2 - anhydroglucose - 3,5,6 - triacetate
- 265. rhamnose triacetate
- 266. glucose pentaacetate
- 267. galactose pentaacetate

Disaccharides

- 268. β - lactose
- 269. α - lactose monohydrate
- 270. maltose
- 271. β - maltose monohydrate
- 272. sucrose
- 273. trehalose
- 274. trehalose dihydrate
- 275. cellobiose
- 276. maltose octaacetate
- 277. cellobiose octaacetate
- 278. lactose octaacetate
- 279. sucrose octaacetate

Trisaccharides and Polysaccharides

- 280. raffinose
- 281. melezitose
- 282. diamylose
- 283. stachyose
- 284. stachyose $2.5 \text{ H}_2\text{O}$
- 285. α - tetramylose
- 286. β - hexamylose
- 287. α - octamylose
- 288. xylan
- 289. diacetyl xylan
- 290. starch hexaacetate

- 291. cellulose hexaacetate
- 292. inulin triacetate
- 293. glycogen
- 294. cellulose
- 295. starch
- 296. inulin
- 297. dextrin

Alkaloids

- 298. morphine monohydrate
- 299. codeine monohydrate
- 300. thebaine
- 301. cinchonine
- 302. cinchonidine
- 303. cinchonamine
- 304. quinine
- 305. papaverine
- 306. quinidine
- 307. strychnine
- 308. narceine
- 309. narceine dihydrate
- 310. brucine
- 311. conine

Aliphatic esters

- 312. methyl formate
- 313. methyl acetate
- 314. methyl propionate
- 315. methyl cinnamate
- 316. methyl oleate
- 317. methyl elaidate

Aromatic esters

- 318. methyl benzoate
- 319. methyl salicylate

Esters of dibasic acids

- 320. dimethyl carbonate
- 321. dimethyl oxalate
- 322. dimethyl malonate
- 323. dimethyl succinate
- 324. dimethyl fumarate
- 325. dimethyl maleate
- 326. dimethyl tartrate (DL)
- 327. dimethyl tartrate (meso)
- 328. dimethyl glutarate
- 329. dimethyl adipate
- 330. dimethyl o - phthalate
- 331. dimethyl m - phthalate
- 332. dimethyl p - phthalate

Glyceryl esters

- 333. 1 - glyceryl monoacetate
- 334. 1,3 - glyceryl diacetate
- 335. glyceryl triacetate
- 336. 1 - glyceryl benzoate
- 337. 2 - glyceryl benzoate
- 338. 1 - glyceryl caprate
- 339. 2 - glyceryl caprate
- 340. tricyclobutylin
- 341. glyceryl tri-n-butyrate
- 342. 1 - glyceryl laurate
- 343. 2 - glyceryl laurate
- 344. 1 - glyceryl myristate
- 345. 2 - glyceryl myristate
- 346. tricyclovalerin
- 347. 1 - glyceryl palmitate
- 348. 2 - glyceryl palmitate
- 349. 1 - glyceryl stearate
- 350. 2 - glyceryl stearate

- 351. glyceryl tribenzoate
- 352. glyceryl trilaurate
- 353. glyceryl trimyristate
- 354. 1,2 - glyceryl dierucate
- 355. 1,2 - glyceryl dibrassidate
- 356. glyceryl trierucate
- 357. glyceryl tribrassidate

Lactones

- 358. levulinic acid lactone
- 359. saccharinic acid lactone
- 360. D - arabonic acid - γ - lactone
- 361. D - galactonic acid - γ - lactone
- 362. D - mannonic acid - γ - lactone
- 363. L - mannonic acid - γ - lactone
- 364. D - gluconic acid - δ - lactone
- 365. D - gluco - α - heptonic acid - γ - lactone
- 366. D - gluco - D - gulo - heptonic acid - γ - lactone
- 367. D - glucaric acid - 3,6 - lactone
- 368. D - glucaric acid - 1,4 - lactone
- 369. D - mannonic acid - 1,4 - 3,6 - dilactone

Aliphatic amides

- 370. formamide
- 371. urea
- 372. guanylurea nitrate
- 373. acetamide
- 374. formyl urea
- 375. oxamide
- 376. malonamide
- 377. oxamic acid

- 378. ethyl carbamate
- 379. hydantoic acid
- 380. propionamide
- 381. guanidine carbonate
- 382. diacetamide
- 383. DL - tartramide
- 384. meso - tartramide
- 385. succinamide

Aromatic amides

- 386. formanilide
- 387. benzamide
- 388. phthalamide
- 389. acetanilide
- 390. phenacetin
- 391. benzanilide

Organic Ring Nitrogen Compounds

- 392. pyridine
- 393. pyridazine
- 394. pyrimidine
- 395. pyrazine
- 396. pyrrole
- 397. piperazine
- 398. pyrrolidine
- 399. α - pyrrolidone
- 400. piperidine
- 401. α - piperidone
- 402. oxindole
- 403. indole
- 404. isatin

- 405. quinoline
- 406. isoquinoline
- 407. skatole
- 408. dipiperidine
- 409. phenazine
- 410. acridine
- 411. lophine
- 412. amarine
- 413. anisine
- 414. amarine hydrate
- 415. tetrazole
- 416. 5 - aminotetrazole
- 417. 5 - hydroxy tetrazole
- 418. 5 - phenyl tetrazole
- 419. imidazole
- 420. pyrazole
- 421. pyrrolaldehyde
- 422. pyrrolaldoxime
- 423. 2,6 - diaminopyridine
- 424. dimethyldiketopiperazine
- 425. benzotriazole
- 426. ϵ - caprolactam
- 427. hexamethylenetetramine
- 428. α - picoline
- 429. β - picoline
- 430. γ - picoline
- 431. picolinic acid
- 432. 2,3 - lutidine
- 433. 2,4 - lutidine

- 434. 3,5 - lutidine
- 435. 2,6 - lutidine
- 436. 3,4 - lutidine
- 437. dipyrryl ketone
- 438. dipyrryl methane
- 439. α - methyl indole
- 440. phyllopyrrole
- 441. 8 - quinolinol
- 442. α - phenyl pyrrole
- 443. N - phenyl pyrrole
- 444. quinaldine
- 445. carbazole
- 446. 3 - aminoacridine
- 447. 5 - aminoacridine
- 448. 2,8 - diaminoacridine
- 449. diphenylfurazan
- 450. isatide
- 451. diphenyloxabiazole
- 452. indigotin
- 453. parabanic acid
- 454. hydantoin
- 455. uramil
- 456. barbituric acid
- 457. 5 - methyl hydantoin
- 458. allantoin
- 459. alloxan
- 460. 5,5 - dimethyl hydantoin
- 461. isouric acid
- 462. methyl allantoin

- 463. pseudouric acid
- 464. dimethyl parabanic acid
- 465. 4 - methyl uracil
- 466. 4 - methylhydrouracil
- 467. 7 - methyl purine
- 468. 7 - methyl hypoxanthine
- 469. theobromine
- 470. alloxantin
- 471. hydurilic acid
- 472. caffeine
- 473. murexide
- 474. veronal
- 475. 4 - phenyl uracil
- 476. amalic acid
- 477. desoxyamalic acid

Organic Ring Oxygen Compounds

- 478. ethylene carbonate
- 479. furan
- 480. tetrahydrofuran
- 481. 1,4 dioxane
- 482. paraldehyde
- 483. tetrahydrofurfuryl alcohol
- 484. furfuryl alcohol
- 485. tetrahydropyran
- 486. furfural
- 487. pyromucic acid
- 488. erythritol diformal
- 489. erythritol diacetal

Porphyrin Compounds

- 490. protoporphyrin
- 491. etioporphyrin (I)
- 492. etioporphyrin (II)
- 493. pyrroporphyrin (XV) monomethyl ester
- 494. rhodoporphyrin (XXI) dimethyl ester
- 495. verdoporphyrin dimethyl ester
- 496. pyropheophorbide a monomethyl ester
- 497. desoxophylloerythrin monomethyl ester
- 498. pheopurpurin 18 monomethyl ester
- 499. phylloerthyryn monomethyl ester
- 500. octaethyl porphyrin
- 501. mesoporphyrin (IX) dimethyl ester
- 502. methyl pheophorbide a
- 503. chlorin p_8 trimethyl ester
- 504. protoporphyrin dimethyl ester
- 505. chloroporphyrin e_8 trimethyl ester
- 506. chlorin e_8 trimethyl ester
- 507. dimethyl pheopurpurin 7
- 508. iso - uroporphyrin (II) octamethyl ester
- 509. γ - phylloporphyrin monomethyl ester
- 510. rhodoporphyrin (XV) dimethyl ester
- 511. coproporphyrin (I) tetramethyl ester
- 512. chloroporphyrin e_8 dimethyl ester
- 513. chlorin e_4 dimethyl ester
- 514. pheoporphyrin a_8 dimethyl ester
- 515. methyl pheophorbide b
- 516. chloroporphyrin e_4 dimethyl ester

Sulfur compounds

- 517. thiourea
- 518. methanethiol
- 519. ethanethiol
- 520. thiolacetic acid
- 521. 2 - thiapropane
- 522. taurine
- 523. thiohydantoin
- 524. β - thiolactic acid
- 525. thiophene
- 526. β , β - dithiolactic acid
- 527. thianthrene

Evaluation of the Combustion Data

The appearance of values for the heats of combustion of organic compounds in the literature as obtained from determinations in a bomb calorimeter with oxygen under pressure can be traced back to the 1880's. International agreement on a chemical standard to be used for the calibration of bomb calorimeters came during the 1920's. The substance chosen was benzoic acid and still today remains as the only chemical primary standard used for this type of calibration. Improvements in calorimetric procedures, measuring instruments, and calculative methods brought the accuracy of the heat of combustion of benzoic acid to 0.01 percent in the 1930's and led Washburn to suggest the need for another refinement in bomb calorimetric calculations. The latter refinement deals with the reduction of combustion data from bomb conditions (certain mass of sample, pressure of oxygen, bomb volume and temperature) to standard conditions in which the reactants and products of the combustion reaction are in their standard states at one atm. pressure. (References to papers dealing with the standard state correction are: (1) E. W. Washburn, J. Res. NBS 10, 525-558 (1933); (2) W. N. Hubbard, D. W. Scott, and G. Waddington, Standard States and Corrections for Combustions in a Bomb at Constant Volume, chapter 5, Experimental Thermochemistry, Vol. I, F. D. Rossini, editor (Interscience Publishers, Inc., New York, 1962); (3) E. J. Prosen, Combustion in a Bomb of Compounds Containing Carbon, Hydrogen, Oxygen and Nitrogen, chapter 6, Experimental Thermochemistry, Vol. I, F. D. Rossini, editor (Interscience Publishers, Inc., New York, 1962)).

As one can imagine from reading the brief chronology of combustion bomb calorimetry in the preceding paragraph, combustion data has

appeared in the literature in a variety of forms and with a variety of corrections. Sometimes the treatment of the data is presented clearly, sometimes not so clearly and sometimes for the reader to guess what the treatment was. We have attempted to bring all pertinent combustion data on organic compounds of interest to a common base by applying the appropriate corrections. The corrections which have been applied when necessary are as follows:

(1) calibration correction

At NBS, standard samples of benzoic acid are purified, the heat of combustion determined, and the combustion value certified under the following conditions: (A) The combustion reaction is referred to 25°C; (B) the sample is burned in a bomb of constant volume in pure oxygen at an initial pressure of 30 atm at 25°C; (C) the number of grams of sample burned is equal to three times the volume of the bomb in liters; (D) the number of grams of water placed in the bomb before combustion is equal to three times the volume of the bomb in liters.

If the value used by an investigator for the heat of combustion of benzoic acid differs significantly from the currently certified value, $-\Delta E_B = 26.434 \pm 0.003 \text{ kJ (mass)}^1$ (weighed in vacuum), a ratio of the appropriate value to that used by the investigator is multiplied by the combustion value under evaluation.

(2) vacuum correction

Particularly, with the earlier literature, the combustion data presented were for the samples weighed in air. From an estimate of the density of a sample, and by assuming a certain temperature, barometric pressure and relative humidity, a buoyancy correction can be applied to reduce the weight of the sample to that in vacuum.

(3) molecular weight correction

Molecular weights are converted to the 1961 table of atomic weights based upon the isotope $C^{12} = 12$.

(4) Washburn correction

This correction reduces bomb calorimetric data from bomb conditions to standard conditions in which the reactants and products are in their standard states at one atmosphere pressure.

(5) ΔnRT correction

The conversion of combustion data presented for the process at constant volume to that at constant pressure is made by means of the equation: $\Delta H = \Delta E + \Delta nRT$.

(6) temperature correction

It is desirable to reduce all combustion data to the reference temperature of 25°C (298.15°K). The appropriate ΔC_p for the combustion reaction must be estimated for the temperature interval under consideration.

(7) calculation of the standard heat of formation

The standard heat of formation of an organic compound is calculated from the standard heat of combustion and the heats of formation of carbon dioxide (g), -94.051 kcal mol⁻¹ and water (l), -68.315 kcal mol⁻¹. (Latter values obtained from D. D. Wagman, W. H. Evans, I. Halow, V. B. Parker, S. M. Bailey and R. H. Schumm, NBS Technical Note 270-3, January, 1968).

(8) units and constants

The evaluated heats of combustion and heats of formation are expressed in kcal mol⁻¹. The unit of energy is the joule and 4.1840 joules equals one calorie. The value of the gas constant, $R = 8.3143 \text{ J deg}^{-1} \text{ mol}^{-1}$. The ice point = 273.15°K.

Alkaloids

	ΔH_c° , 298°K kcal mol ⁻¹	ΔH_f° , 298°K kcal mol ⁻¹	References
conine	-1275.5	-57.6	[1,2]
morphine monohydrate	-2146.1	-170.1	[3,4]
codeine monohydrate	-2327.3	-151.2	[3,5]
thebaine	-2441.3	-63.0	[3,5]
cinchonine	-2545.8	+7.4	[6,7]
cinchonidine	-2545.2	+7.1	[6,7]
cinchonamine	-2596.3	-10.4	[6,7]
cinchonamine nitrate	-2561.0	-79.9	[6,7]
quinine	-2663.7	-37.1	[6,8]
papaverine	-2478.1	-120.2	[3,5]
quinidine	-2662.5	-38.3	[6,8]
strychnine	-2685.5	-41.0	[9,10]
narcotine	-2643.8	-210.9	[3,5]
narceine dihydrate	-2800.9	-421.2	[3,11]
brucine	-2932.7	-118.6	[9,10]

All data tabulated are for substances in the solid phase except conine for which the data refer to the liquid state.

Monosaccharides

	$\Delta H_c^\circ, 298^\circ K$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K$ kcal mol ⁻¹	References
α - D - xylose	-559.0	-252.8	[12,13,14]
β - D - arabinose	-558.8	-253.0	[12,13,15,16, 17]
D - mannose	-672.3	-301.9	[18]
α - D - galactose	-670.1	-304.1	[13,15,16,17, 18,19,20]
D - fucose	-711.5	-262.7	[17]
L - sorbose	-670.6	-303.6	[17,19]
β - L - rhamnose	-717.7	-256.5	[13,17]
α - L - rhamnose monohydrate	-711.2	-331.3	[17]
β - D - fructose	-672.0	-302.2	[17,19,21]
α - methyl - D - glucopyranoside	-841.8	-294.8	[14,23,24,25]
β - methyl - D - glucopyranoside	-840.8	-295.8	[14,24]
β - methyl - D-glucofuranoside	-849.1	-287.5	[24]
D - gluco - α - heptose	-783.1	-353.5	[26]
levo - glucosan	-676.6	-229.3	[13,14,22]
levo - glucosan triacetate	-1303.8	-371.3	[13]
1,2 - anhydroglucose - 3,5,6 - triacetate	-1331.8	-411.7	[13]
rhamnose triacetate	-1544.5	-455.4	[13]
glucose pentaacetate	-1724.2	-532.1	[13]
galactose pentaacetate	-1723.5	-532.8	[13]

All data tabulated are for substances in the solid phase except β - methyl - D - glucofuranoside for which the data refer to the liquid state.

Disaccharides

	$\Delta H_c^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ\text{K}$ kcal mol ⁻¹	References
sucrose	-1348.15	-531.93	[13,15,17,20,25,27-39]
β - lactose	-1350.0	-530.1	[13,15,16,17,19,20,30,31]
α - lactose monohydrate	-1344.6	-603.8	[15,16,17,19,20,21,30,39, 40]
maltose	-1349.3	-530.8	[13,17,20,31,41]
β - maltose monohydrate	-1346.3	-602.1	[17,19,20,21]
trehalose	-1348.8	-531.3	[17]
trehalose dihydrate	-1340.6	-676.1	[17]
cellobiose	-1347.6	-532.5	[13,31]
sucrose octaacetate	-3029.5	-901.9	[13,31]
lactose octaacetate	-3025.4	-906.0	[13]
maltose octaacetate	-3026.9	-904.5	[31]
cellobiose octaacetate	-3028.9	-902.5	[13,31]

All disaccharides listed above are in the solid phase.

Porphyrins

	$\Delta H_c^\circ, 298^\circ K$ kcal mol ⁻¹	$\Delta H_f^\circ, 298^\circ K$ kcal mol ⁻¹	Reference
protoporphyrin	-4238.5	-120.6	[42]
aetioporphyrin (I)	-4305.8	-1.8	[42]
aetioporphyrin (II)	-4312.0	+4.4	[42]
pyrroporphyrin (XV) monomethyl ester	-4150.7	-88.6	[42]
rhodoporphyrin (XXI) dimethyl ester	-4371.8	-123.9	[42]
verdoporphyrin dimethyl ester	-4284.1	-143.3	[42]
pyropheophorbide a monomethyl ester	-4342.6	-84.8	[42]
desoxophylloerythrin monomethyl ester	-4456.8	-38.9	[42]
pheopurpurin 18 monomethyl ester	-4312.5	-114.9	[42]
phylloerthyrin monomethyl ester	-4344.2	-83.2	[42]
octaethyl porphyrin	-4917.2	-39.9	[42]
mesoporphyrin (IX) dimethyl ester	-4624.1	-196.4	[42]
methyl pheophorbide a	-4527.7	-156.1	[42]
chlorin p ₈ trimethyl ester	-4452.9	-299.2	[42]
protoporphyrin dimethyl ester	-4561.7	-122.1	[42]
chloroporphyrin e ₈ trimethyl ester	-4684.2	-230.3	[42]
chlorin e ₈ trimethyl ester	-4693.1	-221.4	[42]
dimethyl pheopurpurin 7	-4600.4	-245.8	[42]
iso-uroporphyrin (II) octamethyl ester	-5738.9	-620.1	[42]
γ - phylloporphyrin monomethyl ester	-4314.4	-87.3	[42]
rhodoporphyrin (XV) dimethyl ester	-4250.3	-245.4	[42]
coproporphyrin (I) tetramethyl ester	-4985.0	-348.3	[42]
chloroporphyrin e ₈ dimethyl ester	-4486.5	-103.3	[42]
chlorin e ₄ dimethyl ester	-4513.2	-144.9	[42]
pheoporphyrin a ₈ dimethyl ester	-4519.5	-164.3	[42]
methyl pheophorbide b	-4414.8	-200.7	[42]
chloroporphyrin e ₄ dimethyl ester	-4503.9	-154.2	[42]

All porphyrins listed above are in the solid phase.

Selection of the Combustion Data

Alkaloids

The selected value for the heat of combustion of each alkaloid is derived from a single investigation.

Monosaccharides

α - D - xylose - The data of Skuratov, Strepikheev, and Kozina [14] were chosen in preference to the earlier work.

β - L - arabinose - The data of Karrer and Fioroni [13] were chosen in preference to the earlier work.

α - D - galactose - The data of Stroh and Fincke [18] were chosen in preference to the earlier work, although the data of Karrer and Fioroni [13] and Stohmann and Langbein [17] are in good agreement with the selection. The data of Clark and Stegeman [19] appear not negative enough.

L - sorbose - The data Clark and Stegeman [19] were chosen in preference to the data of Stohmann and Langbein [17].

β - L - rhamnose - The data of Karrer and Fioroni [13] and Stohmann and Langbein [17] were averaged for the selection.

β - D - fructose - The data of Clark and Stegeman [19] were chosen in preference to the earlier work.

α - methyl - D - glucopyranoside - The data of Skuratov, et al. [14,24] were chosen in preference to other work.

levo - glucosan - The data of Skuratov, et al. [14,24] were chosen in preference to other work.

The remaining monosaccharides not commented on have their selections derived from single investigations.

Disaccharides

sucrose - The data of Verkade and Coops were chosen in preference to other work. The data of Rubner [36], Schl pfer and Fioroni [35], Karrer and Fioroni [13] and Ponomarev and Mlgarskaya [32] are in reasonable agreement with the selection.

  - lactose - The data of Karrer and Fioroni [13,31] and Stohmann and Langbein [17] were averaged for the selection. The more recent work of Clark and Stegeman [19] appears to be not negative enough.

  - lactose monohydrate - The data of Gibson [30], Emery and Benedict [21] and Stohmann and Langbein [17] were averaged for the selection in preference to other work. The more recent work of Clark and Stegeman [19] appears to be too negative.

maltose - The data of Karrer and Fioroni [13,31] and Stohmann and Langbein [17] were averaged for the selection.

  - maltose monohydrate - The data of von Rechenberg [20] appear to be more consistent with the   - lactose and   - lactose monohydrate data, although, this is the oldest work. Stohmann and Langbein [17] determined a value about 8 kcal mol⁻¹ less negative. Emery and Benedict [21] and Clark and Stegeman [19] determined values about 10 kcal mol⁻¹ and 15 kcal mol⁻¹, respectively, more negative than the selection.

The remaining disaccharides not commented on have their selections derived from single investigations.

Porphyrins

The selected values for the heats of combustion of the porphyrin compounds listed were obtained from the data of Stern and Klebs [42].

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