

# NATIONAL BUREAU OF STANDARDS REPORT

9089

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

PROGRESS REPORT FOR THE PERIOD 1 JANUARY TO 31 MARCH 1966

to

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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**NBS PROJECT**

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

George T. Furukawa, Mary K. Buresh, Martin L. Reilly  
George T. Armstrong and Gerald D. Mitchell

Heat Division, Institute for Basic Standards

Progress Report for the Period 1 January to 31 March 1966

to

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Contract No. R-138, Amendment-1

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**U. S. DEPARTMENT OF COMMERCE**  
**NATIONAL BUREAU OF STANDARDS**

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## FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the seventh 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 Heat Division, Institute for Basic Standards (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended 29 April 1965. The program was extended by Amendment 1 for an additional year, beginning 1 July 1965. This report covers the third quarter of the extended contract.

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George T. Armstrong  
Supervisory Chemist  
Project Leader

## 1. Survey and Analysis of Heat-Capacity Data of Some CHNOPS Compounds

George T. Furukawa and Martin L. Reilly

The survey and analysis of heat-capacity data of CHNOPS compounds have been in progress and have been devoted particularly to some important organic compounds. Efforts were made to develop a method for extrapolating to 0°K the heat-capacity data on a number of polyhydroxy compounds which terminate at about 80°K. To date a satisfactory procedure has not been devised. Once a method is found, thermodynamic functions on about eight polyhydroxy substances should be obtained.

The analysis of the heat capacity data of *l*-serine, *l*-methionine, furan, and urea had been completed and tables of thermodynamic properties calculated. These tables are given in Chapter 2.

In the following sections of this chapter are described the sources of data used to obtain the thermodynamic properties. At the beginning of the descriptive text on each compound are given: compound name, structural formula, and molecular weight. The temperature range of the available experimental data is given within the parentheses following the author's names in the descriptive text. The data were analyzed on the IBM 7094 computer. The molal values were calculated using the 1961 atomic weights based on carbon-12. The energy unit, one calorie, is equal to 4.1840 joules.

### 2. Tables of Thermodynamic Functions

#### 2.1 *l*-Serine, HOCH<sub>2</sub>CH(NH<sub>2</sub>)COOH, 105.09414

Hutchens, Cole, and Stout (11-302°K) [6] reported heat-capacity measurements on *l*-serine. The thermodynamic properties given in table 18 are based on the data obtained by Hutchens, et al. No heat of combustion measurements have apparently been available at the time (1964). Hutchens et al. estimated from structural factors  $\Delta H_f^\circ(298^\circ\text{K}) = -173.60 \text{ kcal mol}^{-1}$  and calculated  $\Delta G_f^\circ(298^\circ\text{K}) = -121.6 \text{ kcal mol}^{-1}$ . The value of entropy obtained in table 18 for *l*-serine yields the same result for  $\Delta G_f^\circ(298^\circ\text{K})$ .

#### 2.2 *l*-Methionine, CH<sub>3</sub>SCH<sub>2</sub>CH<sub>2</sub>CH(NH<sub>2</sub>)COOH, 149.21292

Hutchens, Cole, and Stout (11-348°K) [5] determined the heat capacity of *l*-methionine. A transition is shown that extends approximately from 180°K to 350°K with the heat capacity maximum at 305.5°K. Hutchens, et al. estimated the entropy of this transition to be  $4.2 \text{ cal deg}^{-1} \text{ mol}^{-1}$  ( $\sim R \ln 8$ ). Table 19 is based on the data reported by Hutchens, et al.

### 2.3 Furan, CHCHCHCHO, 68.07588

Heat-capacity measurements on furan were reported by Guthrie, et al. (12-300°K) [3]. The measurements shown a  $\lambda$ -point at 56°K, a first-order solid-phase transition at 150°K, and a melting point at 187.55°K. The thermodynamic properties given in table 20 are based on the data obtained by Guthrie, et al. The same authors determined  $\Delta H_f^\circ(298^\circ\text{K})(l) = -14.90 \text{ kcal mol}^{-1}$  and  $\Delta H_f^\circ(298^\circ\text{K})(g) = -8.29 \text{ kcal mol}^{-1}$  from heats of combustion measurements. From statistical thermodynamic calculations, based on rigid-rotator, harmonic-oscillator approximation, and the calorimetric data Guthrie, et al. obtained  $\Delta H_f^\circ$  and  $\Delta G_f^\circ$  for gaseous furan up to 1500°K. The following are some of the values that were reported:

T °K	$-\Delta H_f^\circ$ kcal/mol	$\Delta G_f^\circ$ kcal/mol
298	8.293	0.208
400	9.191	3.258
500	9.872	6.452
800	11.13	16.61

In a more recent paper, Blinc and Pahor [1] described statistical thermodynamic calculations based on new molecular data. Values of  $C_p^\circ$  are shown to be slightly lower than those obtained by Guthrie, et al.

### 2.4 Urea, NH<sub>2</sub>CONH<sub>2</sub>, 60.05583

Measurements of the heat capacity of urea have been reported by the following:

- Gibson, Latimer, and Parks (86-300°K) [2]
- Parks, Huffman, and Barmore (93-298°K) [7]
- Ruehrwein and Huffman (19-318°K) [8]

The more extensive data of Ruehrwein and Huffman were analyzed to obtain the thermodynamic properties given in table 21. Using Huffman's [4] heat of combustion data, Ruehrwein and Huffman obtained  $\Delta H_f^\circ(298^\circ\text{K}) = -79.634 \text{ kcal mol}^{-1}$  and  $\Delta G_f^\circ(298^\circ\text{K}) = -47.118 \text{ kcal mol}^{-1}$ . The  $S^\circ(298^\circ\text{K})$  of table 21 and appropriate recent thermodynamic data yield essentially the same  $\Delta G_f^\circ(298^\circ\text{K})$  as obtained by Ruehrwein and Huffman. The National Bureau of Standards Technical Note 270-1 [9] gives  $\Delta H_f^\circ(298^\circ\text{K}) = -79.56$  and  $\Delta G_f^\circ(298^\circ\text{K}) = -47.04 \text{ kcal mol}^{-1}$ .

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TABLE 18

MOLAL THERMODYNAMIC FUNCTIONS FOR L-SERINE  
 $\text{HOCH}_2\text{CH}(\text{NH}_2)\text{COOH}$   
 2  
 2  
 SOLID PHASE

GRAM MOLECULAR WT. = 105.09414 GRAMS CAL = 4.1840 ABS J  
 $T \text{ DEG K} = 273.15 + T \text{ DEG C}$

T DEG K	$\frac{C_P}{T}$ CAL/DEG	$\frac{H^0 - H^C}{T}$ CAL	$\frac{H^0 - H^C}{T}$ CAL/DEG	$\frac{S^0}{T}$ CAL/DEG	$-\frac{(G^0 - H^C)}{T}$ CAL	$-\frac{(G^0 - H^C)}{T}$ CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.024	0.030	0.006	0.008	0.010	0.002
10.00	0.195	0.487	0.049	0.065	0.162	0.016
15.00	0.646	2.456	0.164	0.218	0.821	0.055
20.00	1.328	7.332	0.367	0.494	2.554	0.128
25.00	2.166	16.013	0.641	0.878	5.943	0.238
30.00	3.112	29.174	0.972	1.356	11.492	0.383
35.00	4.115	47.226	1.349	1.910	19.628	0.561
40.00	5.126	70.330	1.758	2.526	30.694	0.767
45.00	6.126	98.469	2.188	3.187	44.960	0.999
50.00	7.098	131.54	2.631	3.883	62.625	1.252
55.00	8.025	169.37	3.079	4.604	83.834	1.524
60.00	8.916	211.74	3.529	5.341	108.69	1.811
65.00	9.760	258.45	3.976	6.088	137.26	2.112
70.00	10.552	309.25	4.418	6.840	169.58	2.423
75.00	11.306	363.91	4.852	7.594	205.66	2.742
80.00	12.033	422.27	5.278	8.347	245.52	3.069
85.00	12.723	484.17	5.696	9.098	289.13	3.402
90.00	13.371	549.42	6.105	9.844	336.49	3.739
95.00	13.990	617.84	6.504	10.583	387.56	4.080
100.00	14.588	689.29	6.893	11.316	442.31	4.423
105.00	15.166	763.69	7.273	12.042	500.71	4.769
110.00	15.719	840.91	7.645	12.760	562.71	5.116
115.00	16.246	920.83	8.007	13.471	628.30	5.463
120.00	16.756	1003.3	8.361	14.173	697.41	5.812
125.00	17.259	1088.4	8.707	14.867	770.01	6.160
130.00	17.759	1175.9	9.046	15.554	846.07	6.508
135.00	18.255	1266.0	9.378	16.233	925.54	6.856
140.00	18.742	1358.5	9.703	16.906	1008.4	7.203
145.00	19.217	1453.4	10.023	17.572	1094.6	7.549
150.00	19.678	1550.6	10.337	18.231	1184.1	7.894
155.00	20.128	1650.1	10.646	18.884	1276.9	8.238
160.00	20.571	1751.9	10.949	19.530	1372.9	8.581
165.00	21.010	1855.8	11.248	20.170	1472.2	8.922
170.00	21.450	1962.0	11.541	20.804	1574.6	9.262
175.00	21.894	2070.4	11.831	21.432	1680.2	9.601
180.00	22.343	2180.9	12.116	22.055	1788.9	9.938
185.00	22.798	2293.8	12.399	22.673	1900.6	10.274
190.00	23.254	2408.9	12.679	23.287	2015.7	10.609
195.00	23.708	2526.3	12.956	23.897	2133.6	10.942
200.00	24.155	2646.0	13.230	24.503	2254.6	11.273
205.00	24.589	2767.9	13.502	25.105	2378.6	11.603
210.00	25.011	2891.9	13.771	25.703	2505.7	11.932
215.00	25.421	3018.0	14.037	26.296	2635.7	12.259
220.00	25.824	3146.1	14.300	26.885	2768.6	12.585
225.00	26.222	3276.2	14.561	27.470	2904.5	12.909
230.00	26.622	3408.3	14.819	28.050	3043.3	13.232
235.00	27.024	3542.4	15.074	28.627	3185.0	13.553
240.00	27.432	3678.5	15.327	29.200	3329.6	13.873
245.00	27.845	3816.7	15.578	29.770	3477.0	14.192
250.00	28.263	3957.0	15.828	30.337	3627.3	14.509
255.00	28.684	4099.4	16.076	30.901	3780.4	14.825
260.00	29.108	4243.8	16.322	31.462	3936.3	15.140
265.00	29.535	4390.5	16.568	32.021	4095.0	15.453
270.00	29.962	4539.2	16.812	32.577	4256.5	15.765
273.15	30.233	4634.0	16.965	32.926	4359.6	15.961
275.00	30.392	4690.1	17.055	33.130	4420.7	16.075
280.00	30.822	4843.1	17.297	33.682	4587.8	16.385
285.00	31.255	4998.3	17.538	34.231	4757.6	16.693
290.00	31.689	5155.7	17.778	34.778	4930.1	17.000
295.00	32.124	5315.2	18.018	35.324	5105.3	17.306
298.15	32.400	5416.8	18.168	35.667	5217.1	17.498
300.00	32.562	5476.9	18.256	35.867	5283.3	17.611
310.00	33.440	5806.9	18.732	36.949	5647.4	18.217

$H^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG AND 1 ATM PRESSURE.

TABLE 19

MOLAL THERMODYNAMIC FUNCTIONS FOR L-METHIONINE  
 $\text{CH}_3\text{SCH}_2\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$   
 SOLID PHASE

GRAM MOLECULAR WT. = 149.21292 GRAMS CAL = 4.1840 ABS J  
 $T \text{ DEG K} = 273.15 + T \text{ DEG C}$

T	$C_p$	$(H_T^0 - H_0^0)$	$(H_T^0 - H_0^0)/T$	$S_T^0$	$-(G_T^0 - H_0^0)$	$-(G_T^0 - H_0^0)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.062	0.077	0.015	0.021	0.026	0.005
10.00	0.481	1.225	0.122	0.164	0.411	0.041
15.00	1.409	5.744	0.383	0.518	2.019	0.135
20.00	2.746	16.022	0.801	1.100	5.971	0.299
25.00	4.251	33.477	1.339	1.872	13.333	0.533
30.00	5.794	58.581	1.953	2.784	24.925	0.831
35.00	7.328	91.430	2.612	3.793	41.333	1.181
40.00	8.771	131.72	3.293	4.867	62.963	1.574
45.00	10.143	179.03	3.978	5.980	90.068	2.002
50.00	11.445	233.03	4.661	7.117	122.80	2.456
55.00	12.666	293.34	5.333	8.265	161.25	2.932
60.00	13.838	359.62	5.994	9.418	205.46	3.424
65.00	14.960	431.64	6.641	10.570	255.43	3.930
70.00	16.003	509.08	7.273	11.718	311.16	4.445
75.00	16.971	591.52	7.887	12.855	372.59	4.968
80.00	17.968	678.87	8.486	13.982	439.69	5.496
85.00	18.926	771.14	9.072	15.101	512.40	6.028
90.00	19.785	867.95	9.644	16.207	590.68	6.563
95.00	20.602	968.93	10.199	17.299	674.45	7.099
100.00	21.391	1073.9	10.739	18.376	763.64	7.636
105.00	22.160	1182.8	11.265	19.438	858.18	8.173
110.00	22.921	1295.5	11.777	20.487	957.99	8.709
115.00	23.657	1412.0	12.278	21.522	1063.0	9.244
120.00	24.361	1532.0	12.767	22.544	1173.2	9.777
125.00	25.048	1655.6	13.244	23.552	1288.4	10.307
130.00	25.732	1782.5	13.712	24.548	1408.7	10.836
135.00	26.408	1912.9	14.169	25.532	1533.9	11.362
140.00	27.067	2046.6	14.618	26.504	1664.0	11.886
145.00	27.715	2183.5	15.059	27.465	1798.9	12.406
150.00	28.359	2323.7	15.491	28.416	1938.6	12.924
155.00	29.000	2467.1	15.917	29.356	2083.1	13.439
160.00	29.633	2613.7	16.336	30.287	2232.2	13.951
165.00	30.258	2763.4	16.748	31.208	2385.9	14.460
170.00	30.881	2916.3	17.155	32.121	2544.2	14.966
175.00	31.506	3072.2	17.556	33.025	2707.1	15.469
180.00	32.131	3231.3	17.952	33.921	2874.5	15.969
185.00	32.757	3393.5	18.343	34.810	3046.3	16.466
190.00	33.387	3558.9	18.731	35.692	3222.5	16.961
195.00	34.030	3727.4	19.115	36.567	3403.2	17.452
200.00	34.699	3899.2	19.496	37.437	3588.2	17.941
205.00	35.388	4074.4	19.875	38.302	3777.5	18.427
210.00	36.097	4253.1	20.253	39.163	3971.2	18.910
215.00	36.831	4435.4	20.630	40.021	4169.2	19.391
220.00	37.592	4621.5	21.007	40.877	4371.4	19.870
225.00	38.387	4811.4	21.384	41.730	4577.9	20.346
230.00	39.223	5005.4	21.763	42.583	4788.7	20.820
235.00	40.111	5203.7	22.144	43.436	5003.8	21.293
240.00	41.065	5406.6	22.528	44.290	5223.1	21.763
245.00	42.107	5614.5	22.916	45.148	5446.7	22.231
250.00	43.263	5827.9	23.312	46.010	5674.6	22.698
255.00	44.566	6047.4	23.715	46.879	5906.8	23.164
260.00	46.055	6273.9	24.130	47.759	6143.4	23.628
265.00	47.777	6508.3	24.560	48.652	6384.4	24.092
270.00	49.785	6752.1	25.008	49.563	6629.9	24.555
273.15	51.223	6911.2	25.302	50.149	6786.9	24.847
275.00	52.137	7006.8	25.479	50.497	6880.0	25.018
280.00	54.894	7274.2	25.979	51.461	7134.9	25.482
285.00	58.123	7556.5	26.514	52.460	7394.7	25.946
290.00	61.890	7856.3	27.091	53.503	7659.6	26.412
295.00	66.263	8176.4	27.717	54.597	7929.8	26.881
298.15	69.360	8389.9	28.140	55.317	8102.9	27.177
300.00	71.310	8520.0	28.400	55.752	8205.7	27.352
305.00	77.098	8890.7	29.150	56.978	8487.5	27.828
305.50	77.721	8929.4	29.229	57.105	8516.0	27.876
310.00	70.117	9261.4	29.875	58.183	8775.5	28.308
315.00	63.800	9595.3	30.461	59.252	9069.1	28.791
320.00	59.387	9902.5	30.945	60.220	9367.8	29.274
325.00	56.525	10192.	31.359	61.117	9671.2	29.757
330.00	54.864	10470.	31.727	61.966	9978.9	30.239
335.00	54.051	10742.	32.065	62.784	10291.	30.719
340.00	53.736	11011.	32.386	63.582	10607.	31.196
345.00	53.566	11279.	32.694	64.365	10927.	31.671
350.00	53.191	11546.	32.990	65.134	11250.	32.144

$H_0^C$  IS THE ENTHALPY OF THE SOLID AT 0 DEG AND 1 ATM PRESSURE.

TABLE 20

MOLAL THERMODYNAMIC FUNCTIONS FOR FURAN  
C<sub>4</sub>H<sub>4</sub>O

## SOLID AND LIQUID PHASES

GRAM MOLECULAR WT. = 68.07588 GRAMS CAL = 4.1840 ABS J

$$T \text{ DEG K} = 273.15 + T \text{ DEG C}$$

T	C <sub>P</sub>	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>0</sup> )	(H <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>0</sup> )/T	S <sub>T</sub> <sup>0</sup>	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>0</sup> )	-(G <sub>T</sub> <sup>0</sup> -H <sub>0</sub> <sup>0</sup> )/T
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG

## SOLID PHASE I

0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.078	0.097	0.019	0.026	0.032	0.006
10.00	0.597	1.532	0.153	0.205	0.517	0.052
15.00	1.636	6.980	0.465	0.632	2.506	0.167
20.00	2.807	18.082	0.904	1.263	7.180	0.359
25.00	3.965	35.034	1.401	2.015	15.336	0.613
30.00	5.040	57.589	1.920	2.834	27.440	0.915
35.00	6.032	85.308	2.437	3.687	43.733	1.250
40.00	6.913	117.72	2.943	4.551	64.328	1.608
45.00	7.675	154.23	3.427	5.411	89.237	1.983
50.00	8.336	194.30	3.886	6.253	118.35	2.367
55.00	8.922	237.46	4.317	7.076	151.72	2.759
57.50	9.204	260.12	4.524	7.479	169.92	2.955

## LAMBDA TRANSITION

57.50	9.084	260.12	4.524	7.479	169.92	2.955
60.00	9.302	283.11	4.718	7.870	189.11	3.152
65.00	9.699	330.63	5.087	8.631	230.38	3.544
70.00	10.056	380.03	5.429	9.363	275.37	3.934
75.00	10.386	431.15	5.749	10.068	323.96	4.319
80.00	10.689	483.85	6.048	10.748	376.01	4.700
85.00	10.963	537.99	6.329	11.405	431.40	5.075
90.00	11.207	593.43	6.594	12.038	490.02	5.445
95.00	11.430	650.02	6.842	12.650	551.75	5.808
100.00	11.643	707.71	7.077	13.242	616.49	6.165
105.00	11.857	766.46	7.300	13.815	684.14	6.516
110.00	12.078	826.29	7.512	14.372	754.61	6.860
115.00	12.311	887.26	7.715	14.914	827.83	7.199
120.00	12.553	949.42	7.912	15.443	903.73	7.531
125.00	12.803	1012.8	8.102	15.960	982.24	7.858
130.00	13.058	1077.5	8.288	16.467	1063.3	8.179
135.00	13.314	1143.4	8.470	16.965	1146.9	8.496
140.00	13.570	1210.6	8.647	17.454	1233.0	8.807
145.00	13.822	1279.1	8.821	17.935	1321.4	9.113
150.00	14.070	1348.8	8.992	18.407	1412.3	9.415

## SOLID PHASE II

150.00	17.028	1838.0	12.253	21.669	1412.3	9.415
155.00	17.290	1923.8	12.412	22.231	1522.0	9.820
160.00	17.572	2010.9	12.568	22.785	1634.6	10.216
165.00	17.881	2099.6	12.725	23.330	1749.9	10.605
170.00	18.230	2189.8	12.881	23.869	1867.9	10.987
175.00	18.627	2281.9	13.040	24.403	1988.5	11.363
180.00	19.085	2376.2	13.201	24.934	2111.9	11.733
185.00	19.614	2472.9	13.367	25.464	2237.9	12.097
187.55	19.916	2523.3	13.454	25.734	2303.2	12.280

## LIQUID PHASE

187.55	23.816	3432.1	18.300	30.580	2303.2	12.280
190.00	23.843	3490.5	18.371	30.889	2378.5	12.518
195.00	23.907	3609.9	18.512	31.509	2534.5	12.997
200.00	23.982	3729.6	18.648	32.116	2693.5	13.468
205.00	24.067	3849.7	18.779	32.709	2855.6	13.930
210.00	24.162	3970.3	18.906	33.290	3020.6	14.384
215.00	24.269	4091.3	19.029	33.860	3188.5	14.830
220.00	24.386	4213.0	19.150	34.419	3359.2	15.269
225.00	24.514	4335.2	19.268	34.968	3532.6	15.701
230.00	24.652	4458.1	19.383	35.509	3708.8	16.125
235.00	24.800	4581.7	19.497	36.040	3887.7	16.543
240.00	24.959	4706.1	19.609	36.564	4069.2	16.955
245.00	25.127	4831.3	19.720	37.080	4253.3	17.361
250.00	25.304	4957.4	19.830	37.590	4440.0	17.760
255.00	25.490	5084.4	19.939	38.093	4629.2	18.154
260.00	25.685	5212.3	20.047	38.590	4820.9	18.542
265.00	25.888	5341.3	20.156	39.081	5015.1	18.925
270.00	26.098	5471.2	20.264	39.567	5211.7	19.303
273.15	26.234	5553.7	20.332	39.870	5336.8	19.538
275.00	26.315	5602.3	20.372	40.047	5410.8	19.676
280.00	26.538	5734.4	20.480	40.524	5612.2	20.044
285.00	26.767	5867.6	20.588	40.995	5816.0	20.407
290.00	27.000	6002.1	20.697	41.463	6022.1	20.766
295.00	27.237	6137.7	20.806	41.926	6230.6	21.121
298.15	27.388	6223.7	20.874	42.216	6363.1	21.342
300.00	27.478	6274.4	20.915	42.386	6441.4	21.471

H<sub>0</sub><sup>0</sup> IS THE ENTHALPY OF THE SOLID AT 0 DEG AND 1 ATM PRESSURE.

TABLE 21

 MOLAL THERMODYNAMIC FUNCTIONS FOR UREA  
 $\text{NH}_2\text{CONH}_2$   
 SOLID PHASE

GRAM MOLECULAR WT. = 60.05583 GRAMS

CAL = 4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$C_P^C$	$(H_T^0 - H_0^0)$	$(H_T^0 - H_0^0)/T$	$S_T^0$	$-(G_T^0 - H_0^0)$	$-(G_T^0 - H_0^0)/T$
DEG K	CAL/DEG	CAL	CAL/DEG	CAL/DEG	CAL	CAL/DEG
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.021	0.026	0.005	0.007	0.009	0.002
10.00	0.169	0.423	0.042	0.056	0.141	0.014
15.00	0.557	2.122	0.141	0.189	0.712	0.047
20.00	1.212	6.453	0.323	0.434	2.219	0.111
25.00	1.988	14.430	0.577	0.786	5.230	0.209
30.00	2.789	26.363	0.879	1.219	10.216	0.341
35.00	3.580	42.300	1.209	1.709	17.518	0.501
40.00	4.319	62.067	1.552	2.236	27.368	0.684
45.00	5.015	85.423	1.898	2.785	39.914	0.887
50.00	5.653	112.12	2.242	3.347	55.242	1.105
55.00	6.237	141.86	2.579	3.914	73.394	1.334
60.00	6.787	174.44	2.907	4.480	94.380	1.573
65.00	7.284	209.64	3.225	5.044	118.19	1.818
70.00	7.726	247.18	3.531	5.600	144.80	2.069
75.00	8.137	286.85	3.825	6.147	174.18	2.322
80.00	8.537	328.54	4.107	6.685	206.26	2.578
85.00	8.911	372.17	4.378	7.214	241.01	2.835
90.00	9.256	417.60	4.640	7.733	278.38	3.093
95.00	9.573	464.68	4.891	8.242	318.33	3.351
100.00	9.870	513.30	5.133	8.741	360.79	3.608
105.00	10.165	563.38	5.366	9.230	405.72	3.864
110.00	10.463	614.95	5.590	9.709	453.07	4.119
115.00	10.765	668.02	5.809	10.181	502.80	4.372
120.00	11.068	722.61	6.022	10.646	554.87	4.624
125.00	11.369	778.70	6.230	11.104	609.25	4.874
130.00	11.670	836.29	6.433	11.555	665.90	5.122
135.00	11.973	895.40	6.633	12.001	724.79	5.369
140.00	12.277	956.02	6.829	12.442	785.90	5.614
145.00	12.581	1018.2	7.022	12.879	849.21	5.857
150.00	12.886	1081.8	7.212	13.310	914.68	6.098
155.00	13.194	1147.0	7.400	13.738	982.30	6.337
160.00	13.505	1213.8	7.586	14.161	1052.1	6.575
165.00	13.818	1282.1	7.770	14.582	1123.9	6.812
170.00	14.132	1352.0	7.953	14.999	1197.9	7.046
175.00	14.446	1423.4	8.134	15.413	1273.9	7.279
180.00	14.761	1496.4	8.313	15.825	1352.0	7.511
185.00	15.076	1571.0	8.492	16.233	1432.1	7.741
190.00	15.391	1647.2	8.669	16.640	1514.3	7.970
195.00	15.705	1724.9	8.846	17.043	1598.5	8.198
200.00	16.019	1804.2	9.021	17.445	1684.7	8.424
205.00	16.332	1885.1	9.196	17.844	1773.0	8.649
210.00	16.643	1967.6	9.369	18.242	1863.2	8.872
215.00	16.952	2051.5	9.542	18.637	1955.4	9.095
220.00	17.258	2137.1	9.714	19.030	2049.6	9.316
225.00	17.564	2224.1	9.885	19.421	2145.7	9.536
230.00	17.871	2312.7	10.055	19.811	2243.8	9.756
235.00	18.181	2402.8	10.225	20.198	2343.8	9.974
240.00	18.496	2494.5	10.394	20.585	2445.7	10.191
245.00	18.814	2587.8	10.562	20.969	2549.6	10.407
250.00	19.136	2682.7	10.731	21.353	2655.4	10.622
255.00	19.460	2779.2	10.899	21.735	2763.2	10.836
260.00	19.785	2877.3	11.066	22.116	2872.8	11.049
265.00	20.109	2977.0	11.234	22.496	2984.3	11.262
270.00	20.433	3078.4	11.401	22.875	3097.7	11.473
273.15	20.637	3143.1	11.507	23.113	3170.2	11.606
275.00	20.757	3181.4	11.569	23.252	3213.1	11.684
280.00	21.080	3285.9	11.736	23.629	3330.3	11.894
285.00	21.403	3392.2	11.902	24.005	3449.3	12.103
290.00	21.727	3500.0	12.069	24.380	3570.3	12.311
295.00	22.052	3609.4	12.235	24.755	3693.1	12.519
298.15	22.256	3679.2	12.340	24.990	3771.5	12.650
300.00	22.377	3720.5	12.402	25.128	3817.9	12.726
310.00	23.027	3947.5	12.734	25.872	4072.9	13.138
320.00	23.674	4181.0	13.066	26.613	4335.3	13.548

 $H_0^0$  IS THE ENTHALPY OF THE SOLID AT 0 DEG AND 1 ATM PRESSURE.

### 3. Survey of Heats and Free Energies of Formation

In the review of heats and free energies of formation, primary attention was devoted in this period to the inorganic compounds and to organic compounds containing one carbon atom or less. A survey of existing tables of thermodynamic functions was made by reference to prior authoritative compilations. The information found in the survey is summarized in Section 4 of this report. The information is presented in the form of charts in which the occurrence of tabulated data is indicated by coded letters referring to the source. The following functions are listed as headings:

$\Delta H_{fT}^{\circ}$	Enthalpy of formation tabulated as a function of T
$\Delta H_{f298}^{\circ}$	Enthalpy of formation at T = 298°K
$\Delta H_{f0}^{\circ}$	Enthalpy of formation at T = 0°K
$\Delta H_{A0}^{\circ}$	Enthalpy of atomization at T = 0°K
$\Delta H_{A298}^{\circ}$	Enthalpy of atomization at T = 298°K
$\Delta G_{fT}^{\circ}$	Gibbs energy of formation tabulated as a function of T
$\Delta G_{f298}^{\circ}$	Gibbs energy of formation at T = 298°K
log K <sub>p</sub>	Logarithm (base 10) of the equilibrium constant of formation
I.P.	Ionization potential
$\Delta H_{\text{vap}}$	Enthalpy of vaporization
$\Delta H_{\text{fus}}$	Enthalpy of fusion
$\Delta H_{\text{trans}}$	Enthalpy of transition (solid-solid)
$P_T$	Vapor pressure tabulated as a function of T
$H_{298}^{\circ} - H_0^{\circ}$	Enthalpy increment from T = 0°K to T = 298°K
$H_T^{\circ} - H_{298}^{\circ}$	Enthalpy increment above T = 298°K tabulated as a function of T
$H_T^{\circ} - H_0^{\circ}$	Enthalpy increment above T = 0°K tabulated as a function of T
$(H_T^{\circ} - H_0^{\circ})/T$	Enthalpy function, based on T = 0°K, tabulated as a function of T
$(H_T^{\circ} - H_{298}^{\circ})/T$	Enthalpy function, based on T = 298°K, tabulated as a function of T
$G_T^{\circ} - H_0^{\circ}$	Gibbs energy increment above T = 0°K tabulated as a function of T

$G_T^\circ - H_{298}^\circ$	Gibbs energy increment above $T = 298^\circ\text{K}$ tabulated as a function of $T$
$(G_T^\circ - H_{298}^\circ)/T$	Gibbs energy function, based on $T = 298^\circ\text{K}$ , tabulated as a function of $T$
$(G_T^\circ - H_0^\circ)/T$	Gibbs energy function, based on $T = 0^\circ\text{K}$ , tabulated as a function of $T$
$C_p^\circ$	Heat capacity at constant pressure tabulated as a function of $T$
$C_{p298}^\circ$	Heat capacity at constant pressure at $T = 298^\circ\text{K}$
$S_{298}^\circ$	Entropy at $T = 298^\circ\text{K}$
$S_T^\circ$ or $S_T^\circ - S_0^\circ$	Entropy increment above $T = 0^\circ\text{K}$ tabulated as a function of temperature

Some of the above functions give essentially the same information in different ways, as for instance  $(H_T^\circ - H_{298}^\circ)$  and  $(H_T^\circ - H_{298}^\circ)/T$ . However, the various modes of presenting the data are listed separately for the purposes of this survey because the functions are not strictly interchangeable. The sources of data covered thus far in this portion of the study are listed, together with their keyed letters in the first page of Section 4. NBS Circular 500, keyed as letter C, has been searched only through Series I, and has been included only to the extent that data in it has not been superseded by NBS Tech. Note 270-1 (W). Enthalpies of phase changes which are found in Series II have not yet been included, but will be in future summaries.

The compound formulas listed in the left-most column are in strictly alphabetic-numeric order following the scheme used in the Chemical Abstracts Formula Index and in previous reports of this series. Ions were listed if data for them were found. No attempt is made in the charts presented in this report to distinguish the various phases of a compound. Names are given for a few compounds for which the alphabetical formula leaves the nature of the compound unclear.

A cursory scan of the charts in Section 4 shows large vacant areas. They are to be filled in further by additional searches. It is certain that other sources of data will provide additional information, particularly in the columns listed as functions of temperature; however, large gaps are expected to remain after the search has been completed. Structural formulas or names for many of the other compounds can be found by reference to NBS Report 8595 (Table 1, Section 2) or to the sources listed for data.

4. Status of Coverage of Thermodynamic Functions for Inorganic CHNOPS Compounds and Organic CHNOPS Compounds Containing One Carbon Atom per Molecule

Key to Sources of Thermodynamic Functions

- W Wagman, D. C., Evans, W. H., Halow, I, Parker, V. B., Bailey, S. M., and Schumm, R. H., Selected values of chemical thermodynamic properties. Part I. Tables for the first twenty-three elements in the standard order of arrangement. NBS Tech. Note 270-1 (U.S. Government Printing Office, Washington, D. C., October 1965).
- C Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and Jaffe, I., Selected values of chemical-thermodynamic properties. NBS Circular 500 (U. S. Government Printing Office, Washington, D. C., 1952).
- D Dow Chemical Co., (D. R. Stull and collaborators) JANAF Thermochemical Tables, (The Dow Chemical Company, Midland, Michigan, Dec. 31, 1960 to Dec. 31, 1965), available through Supplement 17 as publication PB-168370 (Clearinghouse for Federal Scientific and Technical Information, Washington, D. C., Aug. 1965).
- A Beckett, C. W., and collaborators, NBS Reports as follows:
1. Preliminary report on the thermodynamic properties of lithium, beryllium, magnesium, aluminum and their compounds with oxygen, hydrogen, fluorine, and chlorine.  
NBS Report 6297, January 1959  
NBS Report 6484, July 1959
  2. Preliminary report on the thermodynamic properties of selected light element compounds.  
NBS Report 6645, January 1960  
NBS Report 6928, July 1960
  3. Preliminary report on the thermodynamic properties of selected light-element and some related compounds.  
NBS Report 7093, January 1961  
NBS Report 7192, July 1961  
NBS Report 7437, January 1962  
NBS Report 7587, July 1962  
NBS Report 7796, January 1963  
NBS Report 8033, July 1963  
NBS Report 8186, January 1964  
NBS Report 8504, July 1964  
NBS Report 8628, January 1965  
NBS Report 8919, July 1965  
NBS Report 9028, January 1966

For an explanation of the tables see Section 3 of this report.

Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H$ vap	$\Delta H$ fus	$\Delta H$ trans	$P_T$
C	D	D W A	W A	A	A	D	W	D	A				
C <sup>+</sup>		W	W										
C <sup>+2</sup>		W	W										
C <sup>+3</sup>		W	W										
C <sup>+4</sup>		W	W										
C <sup>+5</sup>		W	W										
C <sup>+6</sup>		W	W										
C <sup>-</sup>	D	D				D		D	A				
CH	D	D W	W			D		D	A				
CH <sup>+</sup>		W	W										
CH <sup>-</sup>									A				
HCN Hydrocyanic Acid	D	D W				D	W	D	A				
HCN Hydrogen Cyanide	W	W	W				W						
HCNO Hydrogen Cyanate	D	D				D		D					
HCNO Cyanic Acid	W						W						



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_{f298}^\circ$	$\Delta H_f^\circ$ O	$\Delta H_{A O}$	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_{f298}^\circ$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	$P_T$
$CH_2O_2$		W					W		A				
$CH_2O_2^+$	W												
$CH_2O_3$		W					W						
$CH_2O_3S$		W											
$CH_2S_3$		W					W						
$CH_3$	D	DW	W			D	W	D	A				
$CH_3^-$									A				
$CH_3NO$		W					W		A				
Methyl- $CH_3NO_2$ nitrite		W											
Nitro- $CH_3NO_2$ methane		W					W		A				
$CH_3N_3$									A				
$CH_3N_3O$		W											
$CH_3N_3O_2$		W											
$CH_3N_3O_3$		W											

Empirical Formula	H <sub>298</sub> <sup>o</sup> H <sub>0</sub>	H <sub>T</sub> <sup>o</sup> H <sub>0</sub>	C <sub>p</sub> <sup>o</sup>	C <sub>p</sub> <sup>o</sup> 298	S <sub>298</sub> <sup>o</sup>	S <sub>T</sub> <sup>o</sup> or S <sub>T-S<sub>0</sub></sub>								
CH <sub>2</sub> O <sub>2</sub>												W	W	
CH <sub>2</sub> O <sub>2</sub> <sup>+</sup>														
CH <sub>2</sub> O <sub>3</sub>													W	
CH <sub>2</sub> O <sub>4</sub> S														
CH <sub>2</sub> S <sub>2</sub>												W	W	
CH <sub>3</sub>														
CH <sub>3</sub> <sup>-</sup>														
CH <sub>3</sub> NO												W	W	
CH <sub>3</sub> NO <sub>2</sub> Nitro-methane												W	W	
CH <sub>3</sub> NO <sub>2</sub> Methyl-nitrite														
CH <sub>3</sub> N <sub>3</sub>														
CH <sub>3</sub> N <sub>3</sub> O <sub>3</sub>														
CH <sub>3</sub> N <sub>3</sub> O <sub>2</sub>														
CH <sub>3</sub> N <sub>3</sub> O <sub>3</sub>														

Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_{f298}^\circ$	$\Delta H_f^\circ$ O	$\Delta H_{A O}$	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$Mf_{298}$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P T
$CH_4$	D	D W	W			D	W	D	A				
$CH_4^+$		W	W										
$CH_4N_2$		W					W						
$CH_4N_2O$ Urea		W					W						
$CH_4N_2O$ Ammonium Cyanate		W	W										
$CH_4N_2S$ Thiourea		W											
$CH_4N_2S$ Ammonium Thiocyanate		W					W						
$CH_4N_4O_2$		W											
$CH_4N_4O_2$ 5-Aminotetrazole Nitrate		W											
$CH_4N_4O_3$ Guanyl-azide Nitrate		W											
$CH_4O$	W	W	W				W		A				
$CH_4O_2$		W											
$CH_4S$		W					W		A				
$CH_5N$		W A					W		A				
$CH_5NO_2$		W					W						



Empirical Formula	$\Delta H_f^\circ$	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ 0	$\Delta H_A$ 0	$\Delta H_A$ 298	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H$ vsp	$\Delta H$ fus	$\Delta H$ trans	$P_T$
$CH_2NO_3$		W					W						
$CH_2N_3$		W											
$CH_2N_3O$		W					W						
$CH_2N_3O_2S$		W											
$CH_2N_3O_5$		W											
$CH_5N^+$		W					W						
$CH_6N_2$		W A	W				W						
$CH_6N_2O_2$		W					W						
$CH_6N_2O_3$		W											
$CH_6N_3O_3$		W											
$CH_7NO$		W					W						
$CH_8N_2O_3$		W					W						
$CH_{12}N_3O_5S$		W											
$CH_{12}O_8$		C											



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ 0	$\Delta H_A$ 0	$\Delta H_A$ 298	$\Delta C_p^\circ$ T	$\Delta C_p^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P. T
$CH_{16}O_6$		C											
CN	D	D				D		D	A				
$CN^-$									A				
$CNO^-$		W					W						
$CNS^-$		W					W						
$CN_4$		W											
$1/n(CN_4)_x$		W											
$CN_4^{0.8}$		W											
CO	D	DW	W			D	W	D	A				
$CO^+$		W	W										
$CO^{+2}$		W	W										
COS	D	DW	W			D	W	D	A				
$CO_2$	D	DW	W			D	W	D	A				
$CO_2^+$		W	W										
$CO_2^-$									A				



Empirical Formula	$\Delta H_f^\circ$	$\Delta H_{f298}$	$\Delta H_f^\circ$	$\Delta H_{A298}$	$\Delta G_f^\circ$	$\Delta G_{f298}$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	$P_T$
$CO_3^{-2}$		W				W						
CP	D	D			D		D					
CS	D	DW			D	W	D					
$CS_2$	D	DW			D	W	D	A				
$C_2$	D	D			D		D	A				
$C_2^-$								A				
$C_2N_2$	D	D			D		D					
$C_3$	D	D			D		D	A				
$C_3^-$								A				
$C_4$	D	D			D		D	A				
$C_4^-$								A				
$C_4N_2$	D	D			D		D					
$C_5$	D	D			D		D					
H	D	DWA	WA	A	D	W	D	A				
$H^+$		W	W	A								



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ 0	$\Delta H_A^\circ$ 0	$\Delta H_A^\circ$ 298	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H$ vap	$\Delta H$ fus	$\Delta H$ trans	$P_T$
$H^-$	D	D W	W			D		D	A				
HN	D	W	W			D		D	A				
HNO	D					D		D					
$HNO_2$	D	W	W			D	W	D					
$HNO_3$	D A	D W A	W			D	W	D					
$HN_2O_2^-$		W											
$HN_3$		W A	W				W		A				
$HN_3^+$		W	W										
HO	D	W D A	W			D	W	D	A				
$HO^-$		W A	W						A				
$HO_2$	D	D W	W			D		D	A				
$HO_2^+$		W	W										
$HO_2^-$		W							A				
$HO_3P^{-2}$		W											
$HC_4^{-2}$		W					W						



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P T
$HO_4S_2^-$							W						
HP	D	D				D		D	D				
HP <sub>2</sub>		C					C						
HP <sub>3</sub>		W											
HS	D	D W	W			D	W	D	A				
HS <sup>-</sup>		W					W		A				
H <sub>2</sub>	D	D W A		A	A	D	W	D	A				
H <sub>2</sub> <sup>+</sup>		W	W										
H <sub>2</sub> N	D	W D A				D		D	A				
H <sub>2</sub> N <sup>-</sup>									A				
H <sub>2</sub> N <sub>2</sub>	D	D				D		D					
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> Nitramide		W											
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> Hyponitrous Acid		W											
H <sub>2</sub> O		W	W						A				
H <sub>2</sub> O <sup>+</sup>									A				



Empirical Formula	$\Delta H_f^\circ$	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ 0	$\Delta H_A$ 0	$\Delta H_A$ 298	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	$P_T$
$H_2O^-$													
$H_2O_2$	D	DWA	W			D	W	D	A				
$H_2O_2^+$		W	W										
$H_2O_2P^-$		W											
$H_2O_3P^-$		W											
$H_2O_4P^-$		W											
$H_2O_4P^{2-}$		W											
$H_2O_7P^{3-}$		W											
$H_2O_3S$		W											
$H_2O_4S$	D	DW				D	W	D					
$H_2O_4S_2$													
$H_2O_6S_2$		W											
$H_2O_7S_2$		W											
$H_2O_8S_2$		W				W							



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P. T
$H_2^P$	D	D				D		D					
$H_2^S$	D	D W	W			D	W	D	A				
$H_2^S$		W											
$H_2^S$		W											
$H_2^S$		W											
$H_2^S$		W											
$H_2^S$		W											
$H_3$									A				
$H_3$	D	D W A	W			D	W	D	A				
$H_3^+$		W	W										
$H_3NO$		W											
$H_3NO^+$		W											
$H_3NO_3^S$		W											
$H_3NO_4$		W		A	A		W						
$H_3N_2$									A				







Empirical Formula	$\Delta H_f^\circ$	$\Delta H_f^\circ$ 1298	$\Delta H_f^\circ$ 0	$\Delta H_f^\circ$ A 0	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 1298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P.T.
$H_4O_5S$		W					W						
$H_4O_5P_2$		W											
$H_4P^+$		W											
$H_4P_2$		W A											
$H_4P_2O_7$		W					W						
$H_5NO$		W					W						
$H_5NO_2$		W					W						
$H_5NS$		W					W						
$H_5NO_3$		W					W						
$H_5NO_4S$		W											
$H_5NO_5S$		W											
$H_5N^+_2$		W											
$H_5N_3O_2$		W											
$H_6NO_2P$		W											
$H_6NO_3P$		W											

Empirical Formula	$\frac{H^0-H^0}{T} 298^0$	$\frac{H^0-H^0}{T} 298$	$\frac{H^0-H^0}{T} 0$	$\frac{H^0-H^0}{T} 298$	$\frac{H^0-H^0}{T}$	$\frac{G^0-H^0}{T} 298$	$\frac{G^0-H^0}{T}$	$\frac{G^0-H^0}{T} 298$	$\frac{G^0-H^0}{T}$	$\frac{C^0-H^0}{T} 298$	$C^0 P$	$C^0 P 298$	$S^0_{298}$	SP or ST 59-50
$H_4O_5S$												W	W	
$H_4O_5P_2$														
$H_4P^+$														
$H_4P_2$														
$H_4P_2O_7$													W	
$H_5NO$									A		A	W A	W A	
$H_5NO_2$													W	
$H_5NS$													W	
$H_5NO_3S$													W	
$H_5NO_5S_2$														
$H_5NO_5S$														
$H_5N^+$													W	
$H_5N_3O_2$														
$H_6NO_2P$														
$H_6NO_3P$														



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^{298}$	$\Delta H_f^\circ$ O	$\Delta H_A^\circ$ O	$\Delta H_{A298}$	$\Delta C_f^\circ$ T	$\Delta C_f^{298}$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P <sub>T</sub>
$H_6N_4O_4P_4$		W											
$H_6N_2O$		W											
$H_6N_2O_4S$		C											
$H_6O_6S$		W											
$H_7NO_6$		W											
$H_7O_8.5P_2$		W											
$H_7NO_7P_2$		W											
$H_8N_2O$													
$H_8N_2O_3S$		W											
$H_8N_2O_3S_2$		W											
$H_8N_2O_4S$		W											
$H_8N_2O_4S_2$		W											
$H_8N_2O_5S_2$		C											
$H_8N_2O_6S$		W											
$H_8N_2O_6S_2$		W											

Empirical Formula	$\Delta H_f^0$	$\Delta H_f^{298}$	$\Delta H_f^0$	$\Delta H_A^0$	$\Delta H_{A298}$	$\Delta G_f^0$	$\Delta f_{298}^0$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P. T.
$H_8N_2O_6S_3$		W											
$H_8N_2O_6S_4$		W											
$H_8N_2O_6S_5$		W											
$H_8N_2O_7S_2$		W											
$H_8N_2O_8S_2$		W					W						
$H_8N_2S$		W					W						
$H_8N_2S_2$		W					W						
$H_8N_2S_3$		W					W						
$H_8N_2S_4$		W					W						
$H_8N_2S_5$		W					W						
$H_8N_2S_8$		W											
$H_8N_4O_2$		W											
$H_8O_7S$		W					W						
$H_9N_2O_3P$		W											
$H_9N_2O_4P$		W					W						



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_A$ 298	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H$ vap	$\Delta H$ fus	$\Delta H$ trans	P. T
$H_{10}N_2O_4S$	W												
$H_{10}N_2O_7P_2$	W						W						
$H_{10}N_4O_4S$	W												
$H_{10}O_8S$	W						W						
$H_{12}N_3O_4P$	W												
$H_{12}N_4O_5S$	W												
$H_{13}N_3O_7P_2$	W						W						
$H_{14}O_6S$	C						C						
$H_{15}O_6P$	C						C						
$H_{16}N_4O_7P_2$	W						W						
$H_{17}N_5O_4S$	W						W						
$H_{18}N_3O_7P$	W												
N	D	DWA	WA	A	A	D	W	D	A				
$N^+$		W	W	A	A				A				
$N^-$									A				



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ 0	$\Delta H_A$ 0	$\Delta H_A$ 298	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	$P_T$
$N^{+2}$		W	W										
$N^{+3}$		W	W										
$N^{+4}$		W	W										
$N^{+5}$		W	W										
$N^{+6}$		W	W										
$N^{+7}$		W	W										
NO	D	W D A	W			D	W	D	A				
$NO^+$		W	W						A				
$NO^-$									A				
$NO_2$	D	W D A	W			D	W	D	A				
$NO_2^-$	D	D W				D	W	D	A				
$NO_3$	D	D W				D	W	D	A				
$NO_3^-$		W					W						
NP	D	D				D		D					
$1/n(NP)_n$		W											

Empirical Formula	$\frac{H^O-H^O}{298}^O$	$\frac{H^O-H^O}{T}^{298}$	$\frac{H^O-H^O}{T}$	$\frac{H^O-H^O}{T}^{298}$	$\frac{CO-H^O}{T}$	$\frac{CO-H^O}{T}^{298}$	$\frac{CO-H^O}{T}$	$\frac{CO-H^O}{T}^{298}$	$C^O_p$	$C^O_p$ 298	$S^O_{298}$	$S^O$ or $S^O_{I-S^O}$
N <sup>+2</sup>												
N <sup>+3</sup>												
N <sup>+4</sup>												
N <sup>+5</sup>												
N <sup>+6</sup>												
N <sup>+7</sup>												
NO		D				D			D		D W	D
NO <sup>+</sup>												
NO <sup>-</sup>												
NO <sub>2</sub>	W	D				D			D	W	D W	D
NO <sub>2</sub> <sup>-</sup>		D				D			D	W	D W	D
NO <sub>3</sub>		D				D			D	W	D W	D
NO <sub>3</sub> <sup>-</sup>										W	W	
NP		D				D			D		D W	D
1/n(NP) <sub>n</sub>												

Empirical Formula	$\Delta H_{fT}^{\circ}$	$\Delta H_{f298}^{\circ}$	$\Delta H_{fO}^{\circ}$	$\Delta H_{AO}$	$\Delta H_{A298}$	$\Delta G_{fT}^{\circ}$	$\Delta G_{f298}^{\circ}$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P <sub>T</sub>
NS	D	D				D		D					
N <sub>2</sub>	D	DWA	WA	A	A	D	W	D	A				
NO <sub>2</sub>	D	DW	W			D	W	D	A				
N <sub>2</sub> O <sub>2</sub> <sup>-2</sup>		W											
N <sub>2</sub> O <sub>3</sub>	D	DWA	W			D	W	D					
N <sub>2</sub> O <sub>4</sub>	D	DW	W			D	W	D					
N <sub>2</sub> O <sub>5</sub>	D	DWA	W			D	W	D					
N <sub>2</sub> O <sub>9</sub> S <sub>2</sub>		W					W						
N <sub>3</sub> <sup>+</sup>		W	W										
N <sub>3</sub> <sup>-</sup>		W	W						A				
N <sub>4</sub>									A				
NS <sub>4</sub>		W											
N <sub>5</sub> P <sub>3</sub>	D	DW				D		D					
O	D	DWA	W	A	A	D	W	D	A				
O <sup>+</sup>		W	W										



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P T
O <sup>+2</sup>		W	W										
O <sup>+3</sup>		W	W										
O <sup>+4</sup>		W	W										
O <sup>+5</sup>		W	W										
O <sup>+6</sup>		W	W										
O <sup>+7</sup>		W	W										
O <sup>+8</sup>		W	W										
O <sup>-</sup>	D	W D	W			D		D	A				
OP	D	D				D	W	D					
OS	D	W D	W			D	W	D	A				
OS <sup>-</sup>									A				
O <sub>2</sub>	D	W D A	W A	A	A	D	W	D	A				
C <sub>2</sub> <sup>+</sup>		W	W						A				
O <sup>-</sup>									A				
O <sub>2</sub> <sup>P</sup>	D	D				D		D					



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_{f298}^\circ$	$\Delta H_f^\circ$ O	$\Delta H_A^\circ$ O	$\Delta H_{A298}^\circ$	$\Delta G_f^\circ$ T	$\Delta G_{f298}^\circ$	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	$P_T$
$O_2S$	D	D W	W			D	W	D	A				
$O_2S^+$		W	W										
$O_3$	D	W D A	W			D	W	D	A				
$O_3^-$									A				
$O_3P^-$		W											
$O_3S$	D	W D	W			D	W	D					
$O_3S^-$		W					W						
$O_3S^{-2}$		W					W						
$O_3S^{-2}$		W											
$O_4$									A				
$O_4P^{-3}$		W					W						
$O_4S^{-2}$		W					W						
$O_4S^{-2}$		W					W						
$O_6P_4$	D	W D				D		D					
$O_6S^{-2}$		W											



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P T
$O_6S_3^{-2}$		W											
$O_6S_4^{-2}$		W											
$O_6S_5^{-2}$		W											
$O_7P_2^{-4}$		W					W						
$O_7S_2^{-2}$		W											
$O_8S_2^{-2}$		W					W						
$O_{10}P_4$	D	DW	W			D	W	D					
P	D	DW	W	A	A	D	W	D	A				
$P^+$				A	A								
$P^-$									A				
PS	D	D				D		D					
$P_2$	D	D				D	W	D	A				
$P_2^-$									A				
$P_2S_3$		W											
$P_4$	D	DW	W			D	W	D	A				



Empirical Formula	$\Delta H_f^\circ$ T	$\Delta H_f^\circ$ 298	$\Delta H_f^\circ$ O	$\Delta H_A^\circ$ O	$\Delta H_{A298}$	$\Delta G_f^\circ$ T	$\Delta G_f^\circ$ 298	Log $K_p$	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P <sub>T</sub>
P <sub>4</sub> S <sub>3</sub>	D	D				D		D					
S	D	DW	W	A	A	D	W	D	A				
S <sup>+</sup>		W	W										
S <sup>-</sup>		W	W						A				
S <sup>+2</sup>		W	W										
S <sup>+3</sup>		W	W										
S <sup>+4</sup>		W	W										
S <sup>+5</sup>		W	W										
S <sup>+6</sup>		W	W										
S <sup>+7</sup>		W	W										
S <sup>+8</sup>		W	W										
S <sup>+9</sup>		W	W										
S <sup>-2</sup>		W					W						
S <sub>2</sub>	D	DW	W			D	W	D	A				
S <sub>2</sub> <sup>+</sup>		W	W										





Empirical Formula	$\Delta H_{fT}^{\circ}$	$\Delta H_{f298}^{\circ}$	$\Delta H_{fO}^{\circ}$	$\Delta H_{AO}$	$\Delta H_{A298}$	$\Delta G_{fT}^{\circ}$	$\Delta G_{f298}^{\circ}$	Log K <sub>p</sub>	I. P.	$\Delta H_{vap}$	$\Delta H_{fus}$	$\Delta H_{trans}$	P <sub>T</sub>
$S_2^{-2}$		W					W						
$S_3$		W											
$S_3^+$		W											
$S_3^{-2}$		W					W						
$S_4$		W											
$S_4^+$		W											
$S_4^{-2}$		W					W						
$S_5$		W											
$S_5^+$		W											
$S_5^{-2}$		W					W						
$S_6$		W											
$S_6^+$		W											
$S_7$		W											
$S_7^+$		W											
$S_8$		DW	W			D	W	D	A				



