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Author
Brewer, Leo

Publication Date
1981-08-01

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Materials & Molecular Research Division

Presented at the Flue Gas Desulfurization Symposium,
Morgantown, WV, November 6-7, 1980

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Leo Brewer

August 1981

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

LBL-11758

Thermodynamic Data for Flue-Gas Desulfurization Processes

Leo Brewer

Materials and Molecular Research Division, Lawrence Berkeley Laboratory and the Department of Chemistry, University of California, Berkeley, CA 94720, U.S.A.

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This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Research, Advanced Environmental Control Division of the U.S. Department of Energy under Contract No. W-7405-ENG-48 through the Morgantown Energy Technology Center, Morgantown, WV.

The efficient design of processes for removal of sulfur dioxide resulting from coal and oil combustion requires thermodynamic and kinetic data for the various materials that might be used in the processes. Examination of the available thermodynamic data for sulfur compounds indicates serious uncertainties and a complete review is planned to provide the best set of internally consistent values obtainable from the literature and from current experiments.

Although the main emphasis will be on information needed for aqueous limestone or lime slurry treatment, the data could also be used for other processes covering a wider temperature range. Thus it is planned to provide the data, when possible, for the range from room temperature to at least 1000K. The present compilation covers most of the materials that might play a role in SO_2 extraction processes and for which data were found. Supplements will be issued as data are obtained for additional substances of interest.

A convenient starting point is the list of recommended values (1) of the report of the CODATA Task Group on key values for thermodynamics, 1977. Some of these values were not considered up-to-date and, as discussed below, appropriate modifications and additions were made to provide what is considered the best set presently available. The present report covers values of ΔH^o_{298}, S^o_{298}, $H^o_{298} - H^o_0$, and C^o_P at

298.15K. Values of $-(G^o-H^o_{298})/RT$ are tabulated for gases and pure condensed phases to allow extension to higher temperatures. The values tabulated have been divided by R so that the data are in proper form for immediate calculation of the equilibrium constants (2) by $\ln K = -\Delta G^o/RT = -\Delta(G^o-H^o_{298})/RT - (\Delta H^o_{298}/R)/T$. As this procedure removes the uncertainty due to R in calculation of heat capacity and entropy values for gases, it was possible to improve the accuracy for some of the atomic species (3). The present compilation, which was prepared for the FGD symposium held at Morgantown, West Virginia on Nov. 6-7, 1980, will be extended to include $-(G^o-H^o_{298})/RT$ values for a range of temperature for the aqueous species in a more complete compilation that will be published as part of the proceedings of the FGD symposium at the American Chemical Society meeting in Atlanta, Georgia, held on March 30-31, 1981.

In such a thermodynamic compilation, it is very important to maintain internal consistency. When older data are replaced by more recent data as has been done here, one must ensure that all other values that depended upon the old data have been changed correspondingly. This is difficult to do and the present compilation is only one step in an iterative process that must be carried out continuously to incorporate newer data. The National Bureau of Standards is uniquely equipped to carry out such a process and it is expected that the Bureau will take over the updating of the data that have been presented here.

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal Research, Advanced Environmental Control Division of the U.S. Department of Energy under Contract Number W-7405-ENG-48 through the Morgantown Energy Technology Center, Morgantown, WV.

TABLE 1

Thermodynamic Properties of Common Gases at 298.15 K

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_p/R
O(g)	29 970 ± 10	19.357 ± 0.002	809.2 ± 0.4	2.635
O_2(g)	0	24.660 ± 0.004	1 044.1 ± 0.5	3.533
O_3(g)	17 100 ± 200	28.733 ± 0.009	1 247 ± 2	4.736
H(g)	26 219 ± 1	13.784 ± 0.001	745.4	2.500
H_2(g)	0	15.704 ± 0.004	1 018.5 ± 0.4	3.468
OH(g)	4 700 ± 100	22.086 ± 0.005	1 060 ± 2	3.594
HO_2(g)	250 ±1000	27.54 ± 0.01	1 203 ± 2	4.198
H_2O	-29 084 ± 5	22.698 ± 0.005	1 192 ± 1	4.042
H_2O_2	-16 340 ± 30	28.193 ± 0.02	1 342 ± 4	5.099
F(g)	9 548 ± 40	19.080 ± 0.002	783.9 ± 0.5	2.736
F_2(g)	0	24.378 ± 0.005	1 061.4 ± 0.5	3.765
HF(g)	-32 870 ± 80	20.887 ± 0.004	1 034.2 ± 0.5	3.504
Cl(g)	14 589 ± 1	19.854 ± 0.002	754.4 ± 0.4	2.627
Cl_2(g)	0	26.817 ± 0.005	1 104 ± 1	4.083
HCl(g)	-11 103 ± 16	22.465 ± 0.004	1 039.2 ± 0.5	3.504
Br(g)	13 457 ± 15	21.036 ± 0.002	745.4	2.500
Br_2(g)	3 718 ± 13	29.509 ± 0.006	1 170 ± 1	4.337
HBr(g)	-4 376 ± 20	23.884 ± 0.004	1 040.1 ± 0.5	3.505

TABLE I (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
I(g)	12 840 ± 2	21.730 ± 0.002	745.4	2.500
I_2(g)	7 508 ± 10	31.339 ± 0.008	1 217 ± 3	4.437
HI(g)	3 187 ± 15	24.834 ± 0.005	1 042.2 ± 0.7	3.507
S(g)	33 360 ± 50	20.172 ± 0.004	800.7 ± 0.5	2.847
S_2(g)	15 520 ± 80	27.429 ± 0.006	1 098 ± 1	3.909
S_3(g)	17 200 ± 400	32.85 ± 0.1	1 400 ± 5	5.78
S_4(g)	16 300 ± 400	35.29 ± 0.1	1 720 ± 5	7.93
S_5(g)	14 900 ± 400	40.6 ± 0.4	2 210 ±20	10.73
S_6(g)	12 100 ± 400	42.55 ± 0.1	2 700 ±10	13.54
S_7(g)	12 900 ± 400	48.1 ± 0.4	3 160 ±20	16.1
S_8(g)	12 020 ± 180	51.20 ± 0.4	3 740 ±20	18.71
HS(g)	16 800 ± 600	23.52 ± 0.01	1 100 ±20	3.90
H_2S(g)	-2 470 ± 80	24.735 ± 0.006	1 198 ± 1	4.11
SO(g)	580 ± 50	26.680 ± 0.002	1 055 ± 5	3.625
SO_2(g)	-35 700 ± 20	29.841 ± 0.007	1 269 ± 2	4.792
SO_3(g)	-47 620 ± 80	30.84 ± 0.01	1 406 ± 2	6.088
SO_4(g)	(-37 000)±2500			
S_2O(g)	-5 400 ± 400	32.10 ± 0.02	1 338 ± 2	5.306
H_2SO_3(g)	(-64 000)±3000	(34.7) ± 1		
H_2SO_4(g)	-88 300 ± 300	35.9 ± 0.3	1 980 ±20	10.1

TABLE I (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
$H_2SO(g)$	-(8 000) ± 2000			
$H_2SO_2(g)$	-(32 000) ± 2000			
$(HO)_2S(g)$	-(33 700) ± 2500	(35.2) ± 0.5		
$HOS(g)$	(2 500) ± 2000	(28.7) ± 0.5		
$HOSO_2(g)$	-(49 000) ± 1500	(33.7) ± 0.5		
$HOSO_3(g)$	-(63 000) ± 1000	(36.2) ± 0.5		
$HOSO_4(g)$	-(57 000) ± 2000			
$(HO)_2S_2O_4(g)$	-(124 000) ± 2500			
$(HO)_2S_2O_5(g)$	-(142 000) ± 1500			
$(HO)_2S_2O_6(g)$	-(137 000) ± 1000	(52) ± 1		
$N(g)$	56 850 ± 50	18.425 ± 0.001	745.4	2.500
$N_2(g)$	0	23.033 ± 0.003	1 042.7 ± 0.1	3.503
$NH(g)$	42 400 ± 1000	21.783 ± 0.002	1 034.5 ± 0.5	3.511
$NH_2(g)$	23 000 ± 1000	23.439 ± 0.006	1 195 ± 1	4.072
$NH_3(g)$	-5 525 ± 40	23.173 ± 0.01	1 208 ± 1	4.285
$NO(g)$	10 980 ± 50	25.334 ± 0.002	1 104.0 ± 1	3.592
$NO_2(g)$	4 110 ± 60	28.872 ± 0.004	1 227.7 ± 2	4.472
$N_2O(g)$	9 810 ± 60	26.448 ± 0.002	1 152.3 ± 1	4.646
$N_2O_3(g)$	10 420 ± 120	37.84 ± 0.04	2 060 ±50	8.75
$N_2O_4(g)$	1 340 ± 120	36.606 ± 0.01	2 014 ± 4	9.52

TABLE I (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
N_2O_5(g)	1 600 ± 180	42.775 ± 0.8	2 500 ± 100	11.46
$ONOSO_2$(g)	-23 100 ± 2000			
HNO(g)	12 270 ± 360	26.557 ± 0.002	1 196 ± 1	4.075
H_2NNO_2	-3 100 ± 1000	32.285 ± 0.1	1 463 ± 10	6.78
HONO(g)	-9 436 ± 70	30.544 ± 0.07	1 395 ± 5	5.57
$HONO_2$(g)	-16 106 ± 70	32.09 ± 0.02	1 430 ± 10	6.51
$HONH_2$(g)	-6 000 ± 1000	28.39 ± 0.3	1 350 ± 90	5.59
$HO(SO_2)NH_2$(g)	-62 400 ± 1000			
$HO(SO_2)ONO$(g)	-64 900 ± 1000			
$HO(SO_2)ONO_2$(g)	-70 000 ± 1500			
C(g)	86 197 ± 60	19.002 ± 0.005	786 ± 1	2.507
CO(g)	-13 294 ± 20	23.761 ± 0.004	1 043 ± 1	3.505
CO_2(g)	-47 329 ± 15	25.700 ± 0.005	1 126 ± 1	4.466
CS(g)	33 460 ± 300	25.311 ± 0.005	1 047 ± 1	3.584
COS(g)	-17 090 ± 200	27.840 ± 0.004	1 194 ± 1	4.991
CS_2(g)	14 070 ± 100	28.61 ± 0.01	1 285 ± 3	5.492
CH_4(g)	-9 000 ± 40	22.389 ± 0.005	1 202 ± 2	4.247
CH_3OH(g)	-24 185 ± 50	28.83 ± 0.02	1 375 ± 2	5.30
CH_2O(g)	-13 060 ± 100	26.30 ± 0.05	1 205 ± 10	4.26
HCOOH(g)	-45 530 ± 75	29.93 ± 0.02	1 314 ± 5	5.494
$(HCOOH)_2$(g)	-98 740 ± 300	40.01 ± 0.5	2 360 ± 100	11.56

TABLE I (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
Mg(g)	17 600 ± 150	17.865 ± 0.001	745.4	2.500
Ca(g)	21 500 ± 150	18.615 ± 0.001	745.4	2.500
Li(g)	19 170 ± 50	16.678 ± 0.002	745.4	2.500
Na(g)	12 880 ± 50	18.475 ± 0.001	745.4	2.500
K(g)	10 730 ± 25	19.271 ± 0.001	745.4	2.500

References to Table I

O(g):(1) except C_p(8); O_2(g):(1,8); O_3(g):(8); H(g):ΔH(1), rest(3); H_2(g):(1) except C_p(8); OH(g):(8,9); HO_2(g):(8,9); H_2O(g):(1) except C_p(8,9) H_2O_2(g):(8); F(g):(1,8); F_2(g):(1) except C_p(8); HF(g):(1,8); Cl(g), Cl_2(g), and HCl(g):(1) except C_p(8); Br(g):ΔH(11), rest(3); Br_2(g) and HBr(g):(1) except C_p(8); I(g):ΔH(11), rest(3); I_2(g):(1) except C_p(8); HI(g):(1,12) except C_p(8); S(g):ΔH(13), rest(1,8); S_2(g): ΔH(10), S_{298}(1,8,9), $H_{298}-H_0$ (9), C_p(8)

S_3(g) to S_8(g):(8). The calculated S_{298} value (8) for S_7(g) using values for fifteen vibrational frequencies agrees closely with the calculation (15) using new determinations of the vibrational frequencies. However Steudel and Schuster (15) point out that Second law treatment of mass spectrometric data (16,17) yield a higher entropy and they suggest addition of a contribution from pseudorotation. Since the number of degrees of freedom beyond translation and rotation is restricted to fifteen, addition of pseudorotation terms would be offset by removal of vibrational contributions. Although there would be a net increase in entropy, the uncertainty of the temperature coefficients of the mass spectrometric measurements is comparable to the difference between Second and Third law values and no consideration of pseudorotation contributions was considered warranted at this time.

References to Table I (continued)

HS(g), H_2S(g), and SO(g):(8,9); SO_2(g):(1) except C_p(8). The S_{298}/R value for SO_2(g) as determined by high-temperature cell measurements (18) is 1.0 lower than the CODATA value (1) and is claimed (18) to be more reliable. However the molecular constants of SO_2 are accurately known (19) and the value calculated using statistical mechanics is much more reliable than the value from cell measurements. SO_3(g):(8); SO_4(g): estimate by (20); S_2O(g):(8); H_2SO_3(g): estimate by (20); H_2SO_4(g):(8,9); H_2SO(g), H_2SO_2(g), HSO(OH)(g), $(HO)_2S$(g), HOS(g), $HOSO_2$(g), HSO_3(g), $HOSO_4$(g), $(HO)_2S_2O_4$(g), $(HO)_2S_2O_5$(g), and $(HO)_2S_2O_6$(g): estimates from (20); N(g):ΔH(1), rest(3); N_2(g):(1,9); NH(g):(8,21); NH_2(g):(8); NH_3(g):(1) except C_p(8); NO(g), NO_2(g), N_2O(g), N_2O_3(g), N_2O_4(g) and N_2O_5(g):(8); $ONOSO_2$(g): estimate by (20); HNO(g), H_2NNO_2(g), HONO(g), $HONO_2$(g), and $HONH_2$(g):(8); $HO(SO_2)NH_2$(g), $HO(SO_2)ONO$(g), and $HO(SO_2)ONO_2$(g): estimates by (20); C(g):(1,9); CO(g) and CO_2(g):(1) except C_p(9); CS(g):(9) except revision of ΔH on basis of (22); COS(g):(9,23); CS_2(g):(9); CH_4(g):(9,23) except ΔH from (24); CH_3OH(g):(25); CH_2O(g):(9) except ΔH from (24); HCOOH(g) and $(HCOOH)_2$:(26); Mg(g) and Ca(g):(3) with ΔH(10,27); Li(g), Na(g), and K(g):(3) with ΔH(10).

TABLE II

Thermodynamic Properties of Solids and Liquids at 298.15 K

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
$H_2O(\ell)$	-34 378 ± 5	8.413 ± 0.01	1 599 ± 2	9.056
$Br_2(\ell)$	0	18.307 ± 0.005	2 950 ± 15	9.102
$I_2(s)$	0	13.968 ± 0.01	1 587 ± 5	6.548
S(orthorhombic)	0	3.855 ± 0.006	530 ± 7	2.730
$H_2SO_4(\ell)$	-97 930 ± 20	18.87 ± 0.01	3 396 ± 10	16.67
$HNO_3(\ell)$	-20 940 ± 60	18.72 ± 0.03	3 285 ± 5	13.215
$NH_4NO_3(s)$	-43 980 ± 35	18.18 ± 0.06	2 846 ± 10	16.728
$NH_4Cl(s)$	-37 900 ± 30	11.41 ± 0.06	1 887 ± 15	10.11
$(NH_4)_2SO_4(s)$	-142 220 ± 60	26.49 ± 0.07	4 252 ± 50	22.55
$NH_2SO_2OH(s)$	-82 500 ± 100			
C(graphite)	0	0.690 ± 0.01	126 ± 2	1.025
Si(s)	0	2.262 ± 0.01	387 ± 1	2.405
SiO_2(α quartz)	-109 530 ± 120	4.987 ± 0.02	832 ± 2	5.36
SiO_2(α crist.)	-109 390 ± 150	5.22 ± 0.02	850 ± 4	5.40

TABLE II (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
Mg(s)	0	3.93 ± 0.01	601 ± 4	2.994
MgO(s)	-72 340 ± 40	3.24 ± 0.02	620 ± 3	4.46
$Mg(OH)_2(s)$	-111 200 ± 100	7.60 ± 0.025	1 372 ± 3	9.26
$MgF_2(s)$	-135 220 ± 150	6.89 ± 0.05	1 193 ± 5	7.407
$MgCl_2(s)$	-77 500 ± 100	10.77 ± 0.1	1 656 ± 10	8.57
$MgCl_2 \cdot 6H_2O(s)$	-300 550 ± 100	44.03 ± 0.5	6 710 ± 25	37.97
Mg(OH)Cl(s)	-96 170 ± 200	10.0 ± 1		8.9
MgS(s)	-41 600 ±1500	6.054 ± 0.05	1 002 ± 5	5.480
$MgSO_3(s)$	-122 080 ± 400	10.4 ± 0.5		
$MgSO_3 \cdot 3H_2O(s)$	-233 140 ± 400	26 ± 1.5		
$MgSO_3 \cdot 6H_2O(s)$	-339 700 ± 400	42 ± 2.5		
$MgSO_4(\alpha)$	-154 900 ± 100	11.0 ± 0.1	1 852 ± 10	11.59
$MgSO_4 \cdot H_2O(s)$	-193 640 ± 100	15.2 ± 0.5	2 660 ± 50	16.1
$MgSO_4 \cdot 6H_2O(s)$	-371 580 ± 100	41.9 ± 0.1	6 665 ± 15	41.9
$MgSO_4 \cdot 7H_2O(s)$	-407 950 ± 80	47.3 ± 0.8	7 470 ± 50	44.8
$MgCO_3(s)$	-131 800 ± 200	7.83 ± 0.03	1 400 ± 4	9.15
$MgCO_3 \cdot 3H_2O(s)$	-237 790 ± 60	23.53 ± 0.08	3 880 ± 20	28.6

TABLE II (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
$MgCO_3 \cdot 5H_2O(s)$	-308 700 ± 400	33.7 ± 1		
$Mg_{3/4}Ca_{1/4}CO_3(s)$	-136 200 ± 50	9.006 ± 0.04	1 515 ± 6	9.32
$Ca(s)$	0	5.00 ± 0.05	689 ± 5	3.12
$CaO(s)$	-76 380 ± 100	4.59 ± 0.04	810 ± 5	5.07
$CaO_2(s)$	-79 600 ± 300	(7.7) ± 0.4		
$CaO_2 \cdot 8H_2O(s)$	-362 800 ± 500			
$Ca(OH)_2(s)$	-118 400 ± 30	10.015 ± 0.07	1 703 ± 8	10.52
$CaF_2(s)$	-146 800 ± 250	8.23 ± 0.05	1 400 ± 8	8.062
$CaCl_2(s)$	-95 700 ± 120	12.58 ± 0.05	1 858 ± 7	8.73
$CaCl_2 \cdot H_2O(s)$	-133 450 ± 200	18.9 ± 0.8		
$CaCl_2 \cdot 2H_2O(s)$	-168 000 ± 150	24.2 ± 1		
$CaCl_2 \cdot 4H_2O(s)$	-240 300 ± 200	34.7 ± 1.5		
$CaCl_2 \cdot 6H_2O(s)$	-312 300 ± 150	47.1 ± 0.9		
$CaClOH(s)$	-109 550 ± 400			
$CaS(s)$	-57 900 ± 350	6.81 ± 0.15	1 082 ± 15	5.71
$CaSO_3(s)$	-139 400 ± 500	12.18 ± 0.15	1 940 ± 20	10.93
$CaSO_3 \cdot \frac{1}{2}H_2O(s)$	-157 400 ± 300	(14.7) ± 0.2	(2 300) ± 100	(14.0)

TABLE II (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_p/R
$CaSO_4$(anhydride)	-172 500 ± 40	12.82 ± 0.07	2 070 ± 20	11.987
$CaSO_4$(sol. α)	-171 430 ± 50	13.03 ± 0.1	2 096 ± 20	12.05
$CaSO_4$(sol. β)	-170 900 ± 50	13.03 ± 0.1	2 091 ± 20	11.91
$CaSO_4\cdot\frac{1}{2}H_2O$(α)	-189 650 ± 50	15.70 ± 0.1	2 480 ± 15	14.36
$CaSO_4\cdot\frac{1}{2}H_2O$(β)	-189 400 ± 50	16.15 ± 0.1	2 544 ± 15	14.93
$CaSO_4\cdot 2H_2O$(s)	-243 280 ± 40	23.33 ± 0.07	3 750 ± 20	22.3
$CaS_2O_3\cdot 4H_2O$(s)	-348 430 ± 500			
$Ca(NO_2)_2$(s)	-89 520 ± 100	(19.8) ± 0.5		
$Ca(NO_3)_2$(s)	-112 840 ± 50	23.25 ± 0.09	3 420 ± 35	17.97
$Ca(NO_3)_2\cdot 2H_2O$(s)	-185 330 ± 130	32.7 ± 1.5		
$Ca(NO_3)_2\cdot 3H_2O$(s)	-220 200 ± 170	37.7 ± 2		
$Ca(NO_3)_2\cdot 4H_2O$(s)	-256 530 ± 140	42.8 ± 2.5		
$CaCO_3$(calcite)	-144 920 ± 50	10.03 ± 0.04	1 740 ± 10	10.04
$CaCO_3\cdot H_2O$(s)	-179 830 ± 100	15.807 ± 0.03		
$CaCO_3\cdot 6H_2O$(s)	-356 200 ± 200	40.214 ± 0.07		
Li(s)	0	3.50 ± 0.02	557 ± 5	2.978
LiOH(s)	-58 625 ± 25	5.15 ± 0.06	892 ± 4	5.965

TABLE II (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_p/R
$LiOH \cdot H_2O(s)$	-95 030 ± 25	8.61 ± 0.06	1 461	9.56
$LiF(s)$	-74 360 ± 40	4.32 ± 0.07	778 ± 3	5.03
$LiCl(s)$	-49 155 ± 25	7.11 ± 0.06	1 119 ± 3	5.776
$Li_2SO_4(s)$	-172 790 ± 45	13.71 ± 0.07	2 240 ± 5	14.145
$Na(s)$	0	6.17 ± 0.02	777 ± 2	3.397
$NaOH(s)$	-51 232 ± 20	7.79 ± 0.06	1 260 ± 4	7.16
$NaOH \cdot H_2O(s)$	-88 370 ± 25	11.93 ± 0.06	1 875 ± 5	10.844
$NaF(s)$	-69 345 ± 40	6.16 ± 0.07	1 021 ± 5	5.635
$NaCl(s)$	-49 470 ± 20	8.66 ± 0.06	1 276 ± 4	6.075
$Na_2S(s)$	-44 000 ±1500	11.6 ± 2		9.96
$Na_2SO_4(s)$	-166 930 ± 40	17.99 ± 0.06	2 790 ± 4	15.308
$Na_2SO_4 \cdot 10H_2O(s)$	-520 560 ± 40	71.15 ± 0.06		69.09
$NaNO_3(s)$	-56 240 ± 30	13.97 ± 0.06	2 071 ± 5	11.19
$Na_2CO_3(s)$	-135 820 ± 30	16.23 ± 0.1	2 503 ± 5	13.29
$Na_2CO_3 \cdot H_2O(s)$	-171 960 ± 30	20.22 ± 0.1	3 168 ± 5	17.51
$Na_2CO_3 \cdot 7H_2O(s)$	-384 700 ± 50	51.3 ± 0.2		
$NaHCO_3(s)$	-114 130 ± 25	12.33 ± 0.15	1 917 ± 4	10.54
$NaCHO_2(s)$	-80 160 ± 50	12.48 ± 0.1	1 896 ± 5	9.94

TABLE II (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	$(H^o_{298}-H^o_0)/R$, K	C^o_P/R
K(s)	0	7.78 ± 0.02	852 ± 2	3.558
KF(s)	-68 520 ± 40	8.00 ± 0.07	1 203 ± 5	5.90
$KF\cdot 2H_2O$(s)	-140 245 ± 40	18.6 ± 0.2		
KCl(s)	-52 473 ± 20	9.97 ± 0.06	1 364 ± 3	6.17
K_2SO_4(s)	-172 900 ± 50	21.12 ± 0.07	3 059 ± 5	15.98
$K_2S_4O_6$(s)	-215 900 ± 600	37.244± 0.04	5 266 ± 5	27.76
KNO_3(s)	-59 395 ± 30	16.00 ± 0.06	2 258 ± 4	11.58

References to Table II

$H_2O(\ell)$:(1) except C_p(9); $Br_2(\ell)$ and $I_2(s)$:(1) except C_p(8); S(orthorhombic):(1) except C_p(8,9), $H_2SO_4(\ell)$: ΔH and S(28), rest (9,27,29); $HNO_3(\ell)$:(23,27); $NH_4NO_3(s)$:(8,30); $NH_4Cl(s)$ and $(NH_4)_2SO_4(s)$: ΔH, S(30), rest (27); $NH_2SO_2OH(s)$:(31); C(graphite): (1,9,23); Si(s):(1) except C_p(23,27); SiO_2 (α quartz):(1) except C_p(9,27); SiO_2(cristobalite): ΔH(32), rest (33); Mg(s):(1) except C_p(10); MgO(s):(1) except C_p (9,27); $Mg(OH)_2(s)$:(27,29); $MgF_2(s)$:(1, 9); $MgCl_2(s)$: ΔH(34), rest (27, 9); $MgCl_2\cdot 6H_2O(s)$, Mg(OH)Cl(s):(27), and MgS(s):(9,57); $MgSO_3(s)$, $MgSO_3\cdot 3H_2O(s)$, and $MgSO_3\cdot 6H_2O(s)$:(27); α $MgSO_4(s)$ and $MgSO_4\cdot H_2O(s)$: (27,76); $MgSO_4\cdot 6H_2O(s)$ and $MgSO_4\cdot 7H_2O$: (27).

$MgCO_3(s)$, $MgCO_3\cdot 3H_2O(s)$, and $MgCO_3\cdot 5H_2O(s)$:(27,35); $Mg_{3/4}Ca_{1/4}CO_3(s)$:(35); Ca(s) and CaO(s):(1,9); $CaO_2(s)$ and $CaO_2\cdot 8H_2O(s)$: (27); $Ca(OH)_2(s)$: ΔH and S (28), rest (9); $CaF_2(s)$, $CaCl_2(s)$ and its hydrates, CaClOH(s), and CaS(s):(27); $CaSO_3$:(36) except H_{298}-H_0 (27); $CaSO_3\cdot \frac{1}{2}H_2O(s)$:(37); $CaSO_4$ and its hydrates: (38); $CaS_2O_3\cdot 4H_2O(s)$ and $Ca(NO_2)_2(s)$:(27); $Ca(NO_3)_2(s)$:ΔH and S (28), rest (27); $Ca(NO_3)_2$ hydrates:(27) with addition of 68K to ΔH/R values to be consistent with Table III; $CaCO_3$ (calcite): ΔH(28), rest (39); $CaCO_3$ hydrates:(27) with addition of 233K to ΔH/R values to be consistent with calcite value;

References to Table II (continued)

Li(s):(1) except C_p(10); LiOH(s), LiOH·H_2O(s), LiF(s) and LiCl(s): ΔH and S (30), rest (9); Li_2SO_4(s):ΔH;ΔS(28), rest (9); Na(s):(1) except C_p(40); NaOH(s), NaOH·H_2O(s), NaF(s), and NaCl(s):(30) except $H_{298}-H_0$ and C_p from (9); Na_2S:(9); Na_2SO_4(s) and $Na_2SO_4 \cdot 10H_2O$(s):ΔH, S(30) with rest (9,41); $NaNO_3$(s):(30) except C_p(57); Na_2CO_3(s):ΔH, S(28,42), rest (9,41); Na_2CO_3(s)·H_2O(s):(42); $Na_2CO_3 \cdot 7H_2O$(s):(40) corrected to agree with (28) and (42) for the other carbonates; $NaHCO_3$(s): (42) except C_p(57); $NaCHO_2$(s):(40); K(s):(1) except C_p(40,57); KF(s):(9,30,40); KF·H_2O(s):(28); KCl(s) and K_2SO_4(s):ΔH and S (30), rest (9,41); $K_2S_4O_6$(s):(37); KNO_3(s):(30) except C_p(57).

TABLE III

Thermodynamic Properties of Aqueous Species at 298.15 K (m/kg for all species)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_P/R
$H_2(aq)$	-486 ± 100	6.9 ± 0.3	21 ± 3
$O_2(aq)$	-1 460 ± 25	13.1 ± 0.1	27 ± 3
$O_3(aq)$	15 100 ± 300	17.8 ± 1	
$H_2O(\ell)$	-34 378 ± 5	8.413 ± 0.01	9.056
H^+	0	0	0
OH^-	-27 666 ± 5	-1.305 ± 0.02	-16.9 ± 0.4
$H_2O_2(aq)$	-22 990 ± 10	17.51 ± 0.03	
HO_2^-	-19 280 ± 200	2.87 ± 0.5	
$O_2^=$	(-4 500) ± 1500	(-5) ± 5	
$HO_2(aq)$	-6 400 ± 1000	17 ± 2	
O_2^-	-6 400 ± 1000	5 ± 4	
$OH(aq)$	-600 ± 300	7.8 ± 1	
O^-	4 500 ± 1000	-2 ± 2	(-14) ± 3
F^-	-40 334 ± 80	-1.67 ± 0.10	-14.1 ± 0.5
$Cl_2(aq)$	-2 500 ± 500	16 ± 1	-10 ± 5
Cl^-	-20 095 ± 10	6.81 ± 0.02	-15.1 ± 0.5
$Br_2(aq)$	-260 ± 100	15.7 ± 0.2	

TABLE III (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_P/R
Br^-	-14 600 ± 20	9.95 ± 0.02	-15.9 ± 0.5
$I_2(aq)$	2 700 ± 50	16.4 ± 0.2	35 ± 4
I^-	-6 830 ± 10	12.80 ± 0.02	-14.5 ± 0.5
I_3^-	-6 300 ± 50	28.5 ± 0.2	0 ± 5
$H_2S(aq)$	-4 600 ±120	15.3 ± 0.4	24 ± 1
HS^-	-1 800 ±120	8.5 ± 0.5	-10 ± 3
$S^=$	4 000 ±2000	-11 ± 5	
$H_2S_2(aq)$	(-6 300)±1500	(20) ± 3	
HS_2^-	(-2 950)±1500	(12) ± 3	
$S_2^=$	3 600 ±1500	(-2) ± 5	
$H_2S_3(aq)$	(-4 800)±1500	(24) ± 3	
HS_3^-	(-1 950)±1500	(16) ± 3	
$S_3^=$	3 100 ±1500	(4) ± 5	
$H_2S_4(aq)$	-4 200 ± 400	(28) ± 3	
HS_4^-	-1 650 ± 400	(20) ± 3	
$S_4^=$	2 600 ± 400	12.4 ± 5	
$H_2S_5(aq)$	-3 450 ± 500	(32) ± 2	
HS_5^-	-1 100 ± 500	(24) ± 2	
$S_5^=$	2 750 ± 500	17 ± 5	
$S_6^=$	2 850 ± 500	(22) ± 5	

TABLE III (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_P/R
$SO_2(aq)$	-38 670 ± 100	20.1 ± 0.4	13.6 ± 2
$H_2SO_3(aq)$	-73 050 ± 100	28.5 ± 0.4	22.7 ± 2
HSO_3^-	-76 000 ± 150	14.4 ± 0.5	(0) ± 4
$S_2O_5^=$	-118 200 ± 600	15 ± 2	
$SO_3^=$	-76 640 ± 450	-4.2 ± 1.5	-40 ± 5
HSO_4^-	-106 560 ± 200	16.2 ± 0.15	-10 ± 6
$SO_4^=$	-109 380 ± 60	2.2 ± 0.1	-33.4 ± 0.8
$H_2S_2O_3(aq)$	-73 150 ± 450	(30) ± 3	
$HS_2O_3^-$	-76 300 ± 400	(18) ± 3	
$S_2O_3^=$	-79 300 ± 360	4 ± 1	-30 ± 1
$S_2O_4^=$	-90 630 ±2000	11 ± 2	
$S_2O_6^=$	-144 100 ±2000	13.4 ± 3	
$S_2O_7^=$	-168 500 ±2000	(24) ± 3	
$S_2O_8^=$	-161 700 ±1000	29.4 ± 2	-13 ± 1
$S_3O_6^=$	-144 300 ±2000	(30) ± 3	
$S_4O_6^=$	-148 700 ± 800	31.3 ± 0.2	-6.1 ± 1.5
$S_5O_6^=$	-148 700 ±2000	(33) ± 3	

TABLE III (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_p/R
$N_2(aq)$	-1 255 ± 100	11.5 ± 0.3	29.6
$NH_3(aq)$	-9 780 ± 25	13.39 ± 0.1	9.0 ± 0.4
$NH_4OH(aq)$	-44 160 ± 25	21.80 ± 0.1	18.1 ± 0.4
NH_4^+	-16 030 ± 30	13.37 ± 0.05	8.3 ± 0.5
$NH_2OH(aq)$	-11 800 ± 400	19.5 ± 1	
NH_3OH^+	-16 070 ± 400	18.6 ± 0.8	
$N_2H_4(aq)$	4 130 ± 20	(16.6) ± 1	
$N_2H_5^+$	-910 ± 100	18 ± 1	8.45± 2
$HNO_2(aq)$	-14 300 ± 100	16.3 ± 1	
NO_2^-	-12 590 ± 100	14.8 ± 0.5	-11 ± 3
NO_3^-	-24 880 ± 50	17.63 ± 0.05	-8.7 ± 0.5
$H_2N_2O_2(aq)$	-7 700 ± 400	26 ± 1	
$HN_2O_2^-$	-6 250 ± 800	17 ± 1	
$N_2O_2^=$	-2 070 ± 800	3 ± 2	
$N_2O(aq)$	7 200 ± 300	14.1 ± 1	22 ± 5
$NO(aq)$	9 550 ± 300	14.3 ± 1	26 ± 5

TABLE III (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_p/R
HCN(aq)	12 880 ± 100	15.3 ± 0.3	
CN^-	18 110 ± 100	11.6 ± 0.3	
HCNO(aq)	-18 800 ± 200	16.1 ± 1	
CNO^-	-17 550 ± 70	12.28 ± 0.5	
HCNS(aq)	11 150 ± 300	(22) ± 1	
CNS^-	9 190 ± 300	17.36 ± 0.2	-4.8 ± 2
CO_2(aq)	-49 704 ± 25	14.36 ± 0.07	25.5 ± 2
H_2CO_3(aq)	-84 080 ± 25	22.77 ± 0.07	34.5 ± 2
HCO_3^-	-82 980 ± 20	11.84 ± 0.07	-6.5 ± 0.5
$CO_3^=$	-81 210 ± 30	-6.01 ± 0.1	-32.9 ± 0.5
CO(aq)	-14 630 ± 60	12.3 ± 0.2	27 ± 3
H_2CO(aq)	-17 300 ± 700	13.3 ± 2	
$H_2C(OH)_2$(aq)	-55 200 ± 700	17.7 ± 2	
H_2COOH^-	-47 600 ±1500	11. ± 3	
HCOOH(aq)	-51 200 ± 50	19.7 ± 0.5	-10 ± 4
$HCOO^-$	-51 220 ± 50	11.0 ± 0.5	-10.6 ± 1

TABLE III (CONTINUED)

	$\Delta H^o_{298}/R$, K	S^o_{298}/R	C^o_p/R
$CH_3COOH(aq)$	-58 410 ± 50	21.5 ± 0.3	20.4 ± 0.3
CH_3COO^-	-58 454 ± 50	10.4 ± 0.3	3.2 ± 0.3
$(COOH)_2(aq)$	-98 040 ± 100	22.5 ± 0.3	
$C_2O_4H^-$	-98 440 ± 100	18.0 ± 0.3	
$C_2O_4^{=}$	-99 250 ± 100	5.49 ± 0.3	
$(CH_2)_2(COOH)_2(aq)$	-109 665 ± 10	(30) ± 2	27.1 ± 0.5
$(CH_2)_2(COO)_2H^-$	-109 260 ± 20	(21.65) ± 2	
$(CH_2)_2(COO)_2^{=}$	-109 200 ± 20	(8.8) ± 2	
$(CH_2)_4(COOH)_2(aq)$	-104 000 ±1000	(38) ± 2	40.4 ± 1
$(CH_2)_4(COO)_2H^-$	-104 200 ±1000	(27.15) ± 2	
$(CH_2)_4(COO)_2^{=}$	-104 520 ±1000	(13.6) ± 2	
Mn^{++}	-26 600 ± 150	-8.15	-1.3 ± 0.4
Mn^{+++}	(-14 000) ± 900		
Fe^{++}	-10 700 ± 100	-16.6 ± 0.3	-0.5 ± 4
Fe^{+++}	-5 840 ± 100	-38 ± 0.5	
Mg^{++}	-56 100 ± 130	-16.6 ± 0.2	-1.9 ± 1
Ca^{++}	-65 270 ± 400	-6.74 ± 0.1	-3.6 ± 1
Li^+	-33 498 ± 10	1.48 ± 0.1	7.3 ± 0.5
Na^+	-28 912 ± 10	7.03 ± 0.02	5.1 ± 0.5
K^+	-30 322 ± 10	12.17 ± 0.02	1.6 ± 0.5

References to Table III

$H_2(aq)$, $O_2(aq)$, and $O_3(aq)$: (43); $H_2O(\ell)$: (1) except C_p(9); OH^-: ΔH (1), S(28), C_p(44,59); $H_2O_2(aq)$ and HO_2^-(23); O_2^-: The Branch and Calvin equation (66) was used to calculate the ionization constant of HO_2^- and the entropy of ionization was estimated. $HO_2(aq)$, O_2^-, OH(aq), and O^-: Baxendale, Ward, and Wardman (67) have reviewed earlier measurements of the ionization constants of HO_2 and OH and have carried out measurements over a range of temperature to obtain the enthalpies and entropies of ionization. They suggested that the enthalpies and entropies of solution would be closely the same for $H_2O_2(g)$ and $HO_2(g)$ and also for $H_2O(g)$ and OH(g). Their suggested procedure was used with the data from Tables I and III to calculate the values tabulated in Table III for $HO_2(aq)$ and OH(aq). Their ionization data were then used to obtain the values for O_2^- and O^-. Their ΔG^o and ΔH^o values for the ionization of OH were shifted slightly to increase S^o/R of O^- from -3 to -2 to better match the value for F^-. The solvation enthalpies of O^- and F^- are almost the same and C_p for O^- was approximated by the value for F^-. F^-: ΔH(1), S(28), C_p(45); $Cl_2(aq)$: (43); Cl^-: ΔH(1), S(28), C_p(46,59); $Br_2(aq)$: Wu et al. (47) treated the solubility of $Br_2(\ell)$ in water as a function of temperature with a correction for deviation from Henry's law to obtain thermodynamic values for $Br_2(aq)$. The difference between their values and the later evaluation of Vasil'ev et al. (48) corresponds to $\ln \gamma_{Br_2} = -(0.689+735/T)m$ or $\gamma_{Br_2} = 0.5$ for $m_{Br_2} = 0.22M$ at 298K which

References to Table III (continued)

seems to be too rapid a deviation from Henry's law. The deviation was reduced to $\ln \gamma_{Br_2} = -0.4m$ yielding $\Delta H^o_{298}/R = -260 \pm 100K$ and $\Delta S^o_{298}/R = -2.6 \pm 0.2$ for $Br_2(\ell) = Br_2(aq)$. Br^-: (28) except C_p(49); I_2(aq): (47,50); I^-: (12) and (28) except C_p(45); I_3^-: Ramette and Sandford (50) have shown that I_5^- and $I_6^{=}$ formation causes errors in the evaluation of thermodynamic values for I_3^- using either I_2 solubility in I^- solutions or calorimetric data with substantial I_2 and I_3^- activities. Johnson (12) has confirmed this effect by demonstrating that the molal enthalpy of solution of I_2 in HI(aq) varies with the amount of I_2 added. The solubility, calorimetric, and spectral measurements have been weighted with regard to influence of I_5^- and $I_6^{=}$ to obtain the values of Table III. H_2S(aq): There have been a number of recent reviews of the solubility of H_2S in water as a function of temperature (43,51,52). The CODATA review (53) has also used calorimetric data to obtain recommended thermodynamic

References to Table III (continued)

values, but their values yield solubilities as much as 13% low between 40 and 260°C. If $\Delta H^{o}_{298}/R$ for solution of H_2S is made 200K more positive, a good fit is obtained but this appears to be too large a shift from the calorimetric determinations and the CODATA $\Delta H^{o}_{298}/R$ value was made only 95K more positive to obtain the values of Table III. HS: In addition to the data considered by CODATA (53), the determination of the first ionization constant of H_2S up to 150°C by Tsonopoulos et al. (54) and the calorimetric measurements by Jordan (55) were used. As noted below in the $S^{=}$ discussion, the tentative second ionization constant accepted by CODATA is believed to be too large by several orders of magnitude and the correction they applied to calorimetric data for hydrolysis of HS^- to $S^{=}$ would be too large. The tentative CODATA values yield for OH^- + $H_2S(g) = HS^- + H_2O$, $\Delta H^{o}_{298}/R$ = -6250K. Jordan (55) has measured the enthalpy of solution of $H_2S(g)$ in 0.1M NaOH and in 0.2M ammonia buffer solutions and has obtained values corresponding to the OH^- reaction between -5890 and -5850K. The dilution correction should be small for this reaction. These values would appear to confirm that the CODATA values for the enthalpy of solution of H_2S and for the first ionization of H_2S should be more positive. As noted above, the CODATA value for the enthalpy of solution was made 95K more positive. The ionization enthalpy was made more positive by 110K resulting in a compromise between the Jordan and CODATA values of -6040±120K.

References to Table III (continued)

$S^=$: The CODATA review (53) notes that reported values of the second ionization constant of H_2S range almost eight orders of magnitude. They selected a tentative value of $\log K_2 = -13$. However, Giggenbach (56) has clearly shown that the ready oxidation of HS^- solutions to polysulfide species has invalidated previous measurements; he demonstrated that $\log K_2$ is at least 1.2 more negative than logK for the ionization of water at all temperatures and is of the order of -17 at 25°C. Tsonopoulos et al. (54) report identical pH titration curves for 0.1M HCl with 0.28M Na_2S or with NaOH. Thus the hydrolysis of $S^=$ must be very complete. They suggest $K_2 = 2 \times 10^{-16}$, but with the $S^=$ concentration so small, they can only set a limit. A value of $\log K_2 = -17 \pm 2$ is used for Table III. The enthalpy and entropy values suggested by Giggenbach were made somewhat more positive. It should be noted that changes in K_1K_2 or changes in ΔG_o and ΔH^o of $S^=$ can be disastrous in calculating the solubilities of metal sulfides if the K_{SP} values are not made consistent with the value of K_1K_2 selected. Whenever K_1K_2 is increased by a factor q, the old value of K_{SP} must be divided by q to maintain the same equilibrium constant or ΔG^o for $MS(s) + 2H^+ = M^{++} + H_2S(g)$. An additional confirmation of the value selected for K_2 of H_2S is given by the recent work of Meyer and Peter (60). They examined the Raman spectrum of HS^- in oxygen-free 1M NaOH and in a solution saturated with solid NaOH. Equal amounts of Na_2S had been added to each

References to Table III (continued)

solution. The HS^- intensity was the same within experimental error in both solutions indicating complete hydrolysis even in a saturated NaOH solution and confirming a pK of at least 17.

The ΔH values given by the NBS (23) for $S_2^=$ and $S_3^=$ were accepted. They are presumably based on the work of Maronny (62). The NBS entropies for $S_4^=$ and $S_5^=$ were also accepted. The remainder of the entropy and enthalpy of formation values were estimated to be consistent with the equilibrium measurements of Schwarenbach and Fischer (61) for HS_4, HS_5, and their ions and with their estimates for HS_2, HS_3, and their ions and the measurements of Boulegue and Michard (72) on $S_4^=$, $S_5^=$, and $S_6^=$. The ΔH values for $S_2^=$ and $S_3^=$ were given a large uncertainty as Schwarzenbach and Fischer report that $S_2^=$ and $S_3^=$ are not detectable in solution and they discredit the cell measurements of Maronny.

SO_2(aq), H_2SO_3(aq): (52); HSO_3^-: Measurements of the ionization constant of sulfurous acid have grouped around 0.017 and 0.013. On the basis of the work of Huss and Eckert (63), 0.014±0.001 was accepted and the thermodynamic values given by Cobble et al. (37) have been revised. Various estimates of C_p^o of HSO_3^- vary from negative to positive; $C_p^o/R = 0 \pm 4$ seems to be the best estimate available at the moment. $S_2O_5^=$: (64); $SO_3^=$: (37), the calorimetric determination of the enthalpy of formation of $SO_3^=$ was given preference to the temperature coefficient of the ionization constant between 5 and 50°C (68); HSO_4^-, $SO_4^=$: (1,28,65) except C_p of $SO_4^=$ (45,73,74,75).

References to Table III (continued)

$H_2S_2O_3$(aq), $HS_2O_3^-$: Ionization constants (71) were combined with $S_2O_3^=$ value of Cobble et al. (37); C_p of $S_2O_3^=$ (73). $S_2O_4^=$, $S_2O_6^=$, $S_2O_7^=$, $S_2O_8^=$, $S_3O_6^=$: (40); C_p of $S_2O_8^=$ (73). $S_4O_6^=$: (37) except for correction of arithmetical error in ΔH calculation. $S_5O_6^=$: (27,40).

N_2(aq):(43); NH_3(aq), NH_4OH(aq), and NH_4^+: New measurements and reviews of earlier values have been presented recently (77-80). The values in Table III are based on the CODATA selections (1,28) for ΔH^o_{298} and S^o_{298} of NH_4^+ with C_p(46,77); NH_2OH(aq) and NH_3OH^+:(23,82,83); N_2H_4(aq) and $N_2H_5^+$:(23,82). HNO_2(aq) and NO_2^-:(23,40); NO_3^-:ΔH(1,28), S(28), C_p(46); $H_2N_2O_2$(aq), $HN_2O_2^-$, $N_2O_2^=$:(40,82); N_2O(aq) and NO(aq):(43); HCN(aq), CN^-, HCNO(aq), and CNO^-:(27); HCNS(aq) and CNS^-:(23,40).

CO_2(aq), H_2CO_3(aq):(42,43); HCO_3^-:(28,42,84) except C_p(45); $CO_3^=$(28,42,85) except C_p(45); CO(aq):(43); H_2CO(aq):(23,87); $H_2C(OH)_2$(aq):(23,27,87); H_2COOH^-:(87); HCOOH(aq):(23,27,86,88); $HCOO^-$:(23,27); CH_3COOH(aq): ΔH and ΔS based on ionization data tabulated by Christensen et al. (86), C_p(77); CH_3COO^-:(40) except C_p(45,77); $(COOH)_2$(aq): Based on ionization data (86); $C_2O_4H^-$ and $C_2O_4^=$:(40). $(CH_2)_2(COOH)_2$(aq):(89,90); $(CH_2)_2(COO)_2H^-$ and $(CH_2)_2(COO)_2^=$:(86); $(CH_2)_4(COOH)_2$(aq):(89,90,91); $(CH_2)_4(COO)_2$-H^- and $(CH_2)_4(COO)_2^=$:(86).

Mn^{++}:(92,93,94); Mn^{+++}(82); Fe^{++} and Fe^{+++}:(95,96), Mg^{++}: ΔH(97), S(29), C_p(45,93,98); Ca^{++}:(28), C_p(93,98); Li^+:(28), C_p(45); Na^+:(28), C_p(46,59); K^+:(28), C_p(46).

TABLE IV Equations for $-(G^o - H^o_{298})/RT$ for 298.15K to T_{max}

Species	T_{max},K	$-(G^o - H^o_{298})/RT =$	Ref.
O(g)	1000	$20.151-7.110\times10^{-3}T+1.9800\times10^{-5}T^2-1.816\times10^{-8}T^3+5.987\times10^{-12}T^4$	(8,9)
O_2(g)	1000	$25.757-9.743\times10^{-3}T+2.6812\times10^{-5}T^2-2.4157\times10^{-8}T^3+7.8845\times10^{-12}T^4$	(8,9)
O_3(g)	1000	$30.370-1.4222\times10^{-2}T+3.8373\times10^{-5}T^2-3.385\times10^{-8}T^3+1.0885\times10^{-11}T^4$	(8)
H(g)	6000	$11.284+2.5[298.15/T-\ln(298.15/T)]$	(3)
H_2(g)	1000	$16.784-9.639\times10^{-3}T+2.6701\times10^{-5}T^2-2.436\times10^{-8}T^3+8.007\times10^{-12}T^4$	(8,9)
OH(g)	1000	$23.170-9.734\times10^{-3}T+2.7076\times10^{-5}T^2-2.4774\times10^{-8}T^3+8.162\times10^{-12}T^4$	(8)
HO_2(g)	1000	$28.909-1.2005\times10^{-2}T+3.2678\times10^{-5}T^2-2.9068\times10^{-8}T^3+9.4155\times10^{-12}T^4$	(8,9)
H_2O(g)	1000	$23.939-1.1055\times10^{-2}T+3.0494\times10^{-5}T^2-2.754\times10^{-8}T^3+9.016\times10^{-12}T^4$	(9)
H_2O_2(g)	1000	$29.901-1.490\times10^{-2}T+4.0313\times10^{-5}T^2-3.5592\times10^{-8}T^3+1.148\times10^{-11}T^4$	(8)
F(g)	1000	$19.906-7.426\times10^{-3}T+2.070\times10^{-5}T^2-1.901\times10^{-8}T^3+6.269\times10^{-12}T^4$	(8)
F_2(g)	1000	$25.601-1.0796\times10^{-2}T+2.9565\times10^{-5}T^2-2.658\times10^{-8}T^3+8.651\times10^{-12}T^4$	(8)
HF(g)	1000	$21.961-9.604\times10^{-3}T+2.6654\times10^{-5}T^2-2.4344\times10^{-8}T^3+8.008\times10^{-12}T^4$	(8)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
$Cl(g)$	1000	$20.695-7.4565\times10^{-3}\ T+2.0567\times10^{-5}\ T^2-1.8693\times10^{-8}\ T^3+6.117\times10^{-12}\ T^4$	(8)
$Cl_2(g)$	1000	$28.130-1.1633\times10^{-2}\ T+3.2008\times10^{-5}\ T^2-2.8973\times10^{-8}\ T^3+9.465\times10^{-12}\ T^4$	(8)
$HCl(g)$	1000	$23.535-9.568\times10^{-3}\ T+2.6541\times10^{-5}\ T^2-2.421\times10^{-8}\ T^3+7.968\times10^{-12}\ T^4$	(8)
$Br(g)$	1000	$21.801-6.842\times10^{-3}\ T+1.899\times10^{-5}\ T^2-1.7341\times10^{-8}\ T^3+5.703\times10^{-12}\ T^4$	(8)
$Br_2(g)$	1000	$30.867-1.2101\times10^{-2}\ T+3.3458\times10^{-5}\ T^2-3.0435\times10^{-8}\ T^3+9.978\times10^{-12}\ T^4$	(8)
$HBr(g)$	1000	$24.950-9.534\times10^{-3}\ T+2.6434\times10^{-5}\ T^2-2.407\times10^{-8}\ T^3+7.914\times10^{-12}\ T^4$	(8)
$I(g)$	1000	$19.230+2.5[298.15/T - \ln(298.15/T)]$	(3)
$I_2(g)$	1000	$32.718-1.2287\times10^{-2}\ T+3.4019\times10^{-5}\ T^2-3.0998\times10^{-8}\ T^3+1.0176\times10^{-11}\ T^4$	(8)
$HI(g)$	1000	$26.090-1.0922\times10^{-2}\ T+2.9862\times10^{-5}\ T^2-2.7574\times10^{-8}\ T^3+9.204\times10^{-12}\ T^4$	(8)
$S(g)$	1000	$21.030-7.725\times10^{-3}\ T+2.1563\times10^{-5}\ T^2-1.9851\times10^{-8}\ T^3+6.556\times10^{-12}\ T^4$	(8,9)
$S_2(g)$	1000	$28.699-1.1222\times10^{-2}\ T+3.0796\times10^{-5}\ T^2-2.7792\times10^{-8}\ T^3+9.067\times10^{-12}\ T^4$	(8,9)
$S_3(g)$	1000	$33.068-4.357\times10^{-3}\ T+1.3802\times10^{-5}\ T^2-6.464\times10^{-9}\ T^3$	(8)
$S_4(g)$	1000	$35.63-6.237\times10^{-3}\ T+1.944\times10^{-5}\ T^2-9.065\times10^{-9}\ T^3$	(8)
$S_5(g)$	1000	$40.99-8.146\times10^{-3}\ T+2.576\times10^{-5}\ T^2-1.207\times10^{-8}\ T^3$	(8)
$S_6(g)$	1000	$47.079-3.984\times10^{-2}\ T+1.0898\times10^{-4}\ T^2-9.8128\times10^{-8}\ T^3+3.1944\times10^{-11}\ T^4$	(8)
$S_7(g)$	1000	$48.644-1.194\times10^{-2}\ T+3.811\times10^{-5}\ T^2-1.791\times10^{-8}\ T^3$	(8)
$S_8(g)$	1000	$51.866-1.381\times10^{-2}\ T+4.416\times10^{-5}\ T^2-2.0755\times10^{-8}\ T^3$	(8)

TABLE IV (CONTINUED)

Species	T_{max},K	$-(G^o - H^o_{298})/RT =$	Ref.
HS(g)	1000	$24.670-1.0438\times10^{-2}\ T+2.9134\times10^{-5}\ T^2-2.6763\times10^{-8}\ T^3+8.849\times10^{-12}\ T^4$	(8,9)
H_2S(g)	1000	$26.031-1.1458\times10^{-2}\ T+3.1424\times10^{-5}\ T^2-2.8197\times10^{-8}\ T^3+9.207\times10^{-12}\ T^4$	(8,9)
SO(g)	1000	$27.844-1.0278\times10^{-2}\ T+2.8161\times10^{-5}\ T^2-2.5297\times10^{-8}\ T^3+8.231\times10^{-12}\ T^4$	(8,9)
SO_2(g)	1000	$31.444-1.4018\times10^{-2}\ T+3.8017\times10^{-5}\ T^2-3.370\times10^{-8}\ T^3+1.0875\times10^{-11}\ T^4$	(8)
SO_3(g)	1000	$32.988-1.8566\times10^{-2}\ T+4.9875\times10^{-5}\ T^2-4.3737\times10^{-8}\ T^3+1.4012\times10^{-11}\ T^4$	(8)
S_2O(g)	1000	$33.876-1.5605\times10^{-2}\ T+4.2477\times10^{-5}\ T^2-3.7926\times10^{-8}\ T^3+1.2285\times10^{-11}\ T^4$	(8)
H_2SO_4(g)	1000	$36.64-9.61\times10^{-3}\ T+2.775\times10^{-5}\ T^2-1.25\times10^{-8}\ T^3$	(8,9)
N(g)	2000	$15.925+2.5[298.15/T - \ln(298.15/T)]$	(3)
N_2(g)	1000	$24.0955-9.506\times10^{-3}\ T+2.6323\times10^{-5}\ T^2-2.3912\times10^{-8}\ T^3+7.849\times10^{-12}\ T^4$	(8,9)
NH(g)	1000	$22.856-9.601\times10^{-3}\ T+2.664\times10^{-5}\ T^2-2.4321\times10^{-8}\ T^3+8.006\times10^{-12}\ T^4$	(8)
NH_2(g)	1000	$24.703-1.1228\times10^{-2}\ T+3.0891\times10^{-5}\ T^2-2.7835\times10^{-8}\ T^3+9.109\times10^{-12}\ T^4$	(8)
NH_3(g)	1000	$24.570-1.2236\times10^{-2}\ T+3.3141\times10^{-5}\ T^2-2.9206\times10^{-8}\ T^3+9.436\times10^{-12}\ T^4$	(8)

TABLE IV (CONTINUED)

Species	T_{max},K	$-(G^o - H^o_{298})/RT =$	Ref.
NO(g)	1000	$26.422-9.721\times10^{-3}\,T+2.6892\times10^{-5}\,T^2-2.4384\times10^{-8}\,T^3+7.997\times10^{-12}\,T^4$	(8)
NO_2(g)	1000	$30.359-1.299\times10^{-2}\,T+3.518\times10^{-5}\,T^2-3.109\times10^{-8}\,T^3+1.0026\times10^{-11}\,T^4$	(8)
N_2O(g)	1000	$28.028-1.378\times10^{-2}\,T+3.7298\times10^{-5}\,T^2-3.3014\times10^{-8}\,T^3+1.0655\times10^{-11}\,T^4$	(8)
N_2O_3(g)	1000	$38.17-6.50\times10^{-3}\,T+2.054\times10^{-5}\,T^2-9.474\times10^{-9}\,T^3$	(8)
N_2O_4(g)	1000	$39.99-2.927\times10^{-2}\,T+7.86\times10^{-5}\,T^2-6.898\times10^{-8}\,T^3+2.212\times10^{-11}\,T^4$	(8)
N_2O_5(g)	1000	$43.42-9.960\times10^{-3}\,T+2.970\times10^{-5}\,T^2-1.357\times10^{-8}\,T^3$	(8)
HNO(g)	1000	$27.831-1.126\times10^{-2}\,T+3.077\times10^{-5}\,T^2-2.740\times10^{-8}\,T^3+8.903\times10^{-12}\,T^4$	(8)
H_2NNO_2(g)	1000	$32.87-7.224\times10^{-3}\,T+1.994\times10^{-5}\,T^2-8.743\times10^{-9}\,T^3$	(8)
HONO(g)	1000	$30.86-4.853\times10^{-3}\,T+1.441\times10^{-5}\,T^2-6.523\times10^{-9}\,T^3$	(8)
$HONO_2$(g)	1000	$34.517-2.077\times10^{-2}\,T+5.519\times10^{-5}\,T^2-4.788\times10^{-8}\,T^3+1.5255\times10^{-11}\,T^4$	(8)
$HONH_2$(g)	1000	$28.77-5.215\times10^{-3}\,T+1.504\times10^{-5}\,T^2-6.675\times10^{-9}\,T^3$	(8)

TABLE IV (CONTINUED)

Species	T_{max},K	$-(G^o - H^o_{298})/RT =$	Ref.
C(g)	1000	$19.772-6.884\times10^{-3}T+1.9091\times10^{-5}T^2-1.7432\times10^{-8}T^3+5.728\times10^{-12}T^4$	(9)
CO(g)	1000	$24.825-9.523\times10^{-3}T+2.6363\times10^{-5}T^2-2.3935\times10^{-8}T^3+7.858\times10^{-12}T^4$	(9)
CO_2(g)	1000	$27.229-1.331\times10^{-2}T+3.5974\times10^{-5}T^2-3.177\times10^{-8}T^3+1.024\times10^{-11}T^4$	(9)
CS(g)	1000	$26.455-1.0117\times10^{-2}T+2.7736\times10^{-5}T^2-2.4947\times10^{-8}T^3+8.130\times10^{-12}T^4$	(9)
COS(g)	1000	$29.542-1.4862\times10^{-2}T+4.029\times10^{-5}T^2-3.5768\times10^{-8}T^3+1.1556\times10^{-11}T^4$	(9)
CS_2(g)	1000	$30.460-1.6203\times10^{-2}T+4.4067\times10^{-5}T^2-3.9307\times10^{-8}T^3+1.2733\times10^{-11}T^4$	(9)
CH_4(g)	1000	$23.829-1.243\times10^{-2}T+3.3115\times10^{-5}T^2-2.841\times10^{-8}T^3+9.068\times10^{-12}T^4$	(9)
CH_3OH(g)	1000	$30.656-1.5764\times10^{-2}T+4.151\times10^{-5}T^2-3.5265\times10^{-8}T^3+1.1145\times10^{-11}T^4$	(25)
CH_2O(g)	1000	$26.55-3.707\times10^{-3}T+1.083\times10^{-5}T^2-4.76\times10^{-9}T^3$	(9)
HCOOH(g)	1000	$32.052-1.8039\times10^{-2}T+4.7926\times10^{-5}T^2-4.1987\times10^{-8}T^3+1.370\times10^{-11}T^4$	(26)
$(HCOOH)_2$(g)	1000	$40.97-1.198\times10^{-2}T+3.327\times10^{-5}T^2-1.45\times10^{-8}T^3$	(26)
Mg(g)	2000	$15.365+2.5[298.15/T - \ln(298.15/T)]$	(3)
Ca(g)	1500	$16.115+2.5[298.15/T - \ln(298.15/T)]$	(3)
Li(g)	1600	$14.178+2.5[298.15/T - \ln(298.15/T)]$	(3)
Na(g)	1700	$15.975+2.5[298.15/T - \ln(298.15/T)]$	(3)
K(g)	1400	$16.771+2.5[298.15/T - \ln(298.15/T)]$	(3)

Table IV (continued)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
$H_2O(\ell)$	500	$18.025-8.867\times10^{-2}\,T+2.8856\times10^{-4}\,T^2-3.9505\times10^{-7}\,T^3+2.08\times10^{-10}\,T^4$	(9)
$Br_2(\ell)$	500	$22.845-3.628\times10^{-2}\,T+8.841\times10^{-5}\,T^2-5.95\times10^{-8}\,T^3$	(8)
$I_2(s)$	387	$15.897-1.333\times10^{-2}\,T+2.30\times10^{-5}\,T^2$	(8)
$I_2(\ell)$	760	$-45.946+1204.8/T+9.569\ln T$	(8)
S(ortho-rhombic)	400	$4.50-4.58\times10^{-3}\,T+8.11\times10^{-6}\,T^2$	(8,9)
S(mono-clinic)	400	$4.27-3.69\times10^{-3}\,T+7.39\times10^{-6}\,T^2$	(8,9)
$S(\ell)$	1000	$2.614+2.667\times10^{-3}\,T+2.592\times10^{-6}\,T^2-1.67\times10^{-9}\,T^3$	(8)
$H_2SO_4(\ell)$	700	$23.435-3.773\times10^{-2}\,T+8.96\times10^{-5}\,T^2-4.856\times10^{-8}\,T^3$	(9)
$HNO_3(\ell)$	350	$5.505+13.215[298.15/T - \ln(298.15/T)]$	(27)
$NH_4NO_3(s)$	450	$21.94-2.623\times10^{-2}\,T+4.086\times10^{-5}\,T^2+1.59\times10^{-8}\,T^3$	(8)
$NH_4NO_3(\ell)$	900	$-108.40+4468/T+19.364\ln T$	(8)
$NH_4Cl(s)$	500	$17.59-4.927\times10^{-2}\,T+1.204\times10^{-4}\,T^2-8.27\times10^{-8}\,T^3$	(57)
$(NH_4)_2SO_4(s)$	600	$17.61-3.44\times10^{-2}\,T+8.164\times10^{-5}\,T^2-4.86\times10^{-8}\,T^3$	(57)

TABLE IV (CONTINUED)

Species	T_{max},K	$-(G^o - H^o_{298})/RT =$	Ref.
C(graphite)	1000	$1.125-3.593 \times 10^{-3} T+9.165 \times 10^{-6} T^2-7.424 \times 10^{-9} T^3+2.249 \times 10^{-12} T^4$	(9)
Si(s)	1000	$3.095-7.270 \times 10^{-3} T+1.976 \times 10^{-5} T^2-1.766 \times 10^{-8} T^3+5.73 \times 10^{-12} T^4$	(9)
SiO_2(α,β quartz)	1000	$6.94 -1.682 \times 10^{-2} T+4.48 \times 10^{-5} T^2-3.88 \times 10^{-8} T^3+1.236 \times 10^{-11} T^4$	(9)
SiO_2(α,β crist.)	1000	$7.60 -1.975 \times 10^{-2} T+5.146 \times 10^{-5} T^2-4.445 \times 10^{-8} T^3+1.396 \times 10^{-11} T^4$	(33)
Mg(s)	922	$4.88 -8.405 \times 10^{-3} T+2.308 \times 10^{-5} T^2-2.076 \times 10^{-8} T^3+6.80 \times 10^{-12} T^4$	(9)
MgO(s)	1000	$4.85 -1.398 \times 10^{-2} T+3.77 \times 10^{-5} T^2-3.342 \times 10^{-8} T^3+1.077 \times 10^{-11} T^4$	(9)
$Mg(OH)_2$(s)	600	$10.91 -2.664 \times 10^{-2} T+6.355 \times 10^{-5} T^2-3.85 \times 10^{-8} T^3$	(57)
MgF_2(s)	1000	$7.25 -6.14 \times 10^{-3} T+1.872 \times 10^{-5} T^2-8.66 \times 10^{-9} T^3$	(9)
$MgCl_2$(s)	990	$11.06 -6.19 \times 10^{-3} T+1.993 \times 10^{-5} T^2-9.34 \times 10^{-9} T^3$	(9)
$MgCl_2 \cdot 6H_2O$(s)	385	$44.03 +1.3 \times 10^{-4}(T - 298.15)^2$	(41,57)
MgOHCl(s)	850	$5.49 -5.09 \times 10^{-3} T+1.37 \times 10^{-5} T^2+6.6 \times 10^{-9} T^3$	(57)

TABLE IV (CONTINUED)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
MgS(s)	1000	$6.22 - 3.83 \times 10^{-3}\ T + 1.248 \times 10^{-5}\ T^2 - 5.87 \times 10^{-9}\ T^3$	(9)
$MgSO_4$(s)	1000	$11.67 - 1.025 \times 10^{-2}\ T + 3.031 \times 10^{-5}\ T^2 - 1.367 \times 10^{-8}\ T^3$	(9)
$MgSO_4 \cdot H_2O$(s)	320	$15.2 + 8 \times 10^{-5} (T - 298.15)^2$	(27)
$MgSO_4 \cdot 6H_2O$(s)	320	$41.9 + 1 \times 10^{-4} (T - 298.15)^2$	(57)
$MgSO_4 \cdot 7H_2O$(s)	320	$47.3 + 2 \times 10^{-4} (T - 298.15)^2$	(57)
$MgCO_3$(s)	1000	$9.05 - 1.228 \times 10^{-2}\ T + 3.172 \times 10^{-5}\ T^2 - 1.496 \times 10^{-8}\ T^3$	(9)
$MgCO_3 \cdot 3H_2O$(s)	320	$23.53 + 1 \times 10^{-4} (T - 298.15)^2$	(27)
Ca(s)	721	$5.49 - 4.67 \times 10^{-3}\ T + 1.20 \times 10^{-5}\ T^2 - 6.38 \times 10^{-9}\ T^3$	(9)
CaO(s)	1000	$4.82 - 4.07 \times 10^{-3}\ T + 1.26 \times 10^{-5}\ T^2 - 5.86 \times 10^{-9}\ T^3$	(9)
$Ca(OH)_2$(s)	1000	$13.73 - 3.24 \times 10^{-2}\ T + 8.79 \times 10^{-5}\ T^2 - 7.846 \times 10^{-8}\ T^3 + 2.544 \times 10^{-11}\ T^4$	(9)

TABLE IV (CONTINUED)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
$CaF_2(s)$	1000	$10.97 - 2.416 \times 10^{-2}\ T + 6.62 \times 10^{-5}\ T^2 - 5.967 \times 10^{-8}\ T^3 + 1.95 \times 10^{-11}\ T^4$	(9)
$CaCl_2(s)$	1000	$15.39 - 2.49 \times 10^{-2}\ T + 6.862 \times 10^{-5}\ T^2 - 6.224 \times 10^{-8}\ T^3 + 2.04 \times 10^{-11}\ T^4$	(9)
$CaS(s)$	1000	$6.97 - 3.93 \times 10^{-3}\ T + 1.285 \times 10^{-5}\ T^2 - 6.05 \times 10^{-9}\ T^3$	(9)
$CaSO_3(s)$	1000	$12.75 - 9.16 \times 10^{-3}\ T + 2.75 \times 10^{-5}\ T^2 - 1.236 \times 10^{-8}\ T^3$	(36)
$CaSO_3 \cdot \frac{1}{2}H_2O(s)$	320	$14.7 + 7 \times 10^{-5}(T - 298.15)^2$	(37)
$CaSO_4$ (anhydride)	1000	$13.31 - 9.10 \times 10^{-3}\ T + 2.8245 \times 10^{-5}\ T^2 - 1.246 \times 10^{-8}\ T^3$	(38)
$CaSO_4$ (sol α)	320	$13.03 + 5.8 \times 10^{-5}(T - 298.15)^2$	(38)
$CaSO_4$ (sol β)	320	$13.03 + 5.7 \times 10^{-5}(T - 298.15)^2$	(38)
$CaSO_4 \cdot \frac{1}{2}H_2O(\alpha)$	450	$24.74 - 7.22 \times 10^{-2}\ T + 1.778 \times 10^{-4}\ T^2 - 1.253 \times 10^{-7}\ T^3$	(38)
$CaSO_4 \cdot \frac{1}{2}H_2O(\beta)$	450	$25.63 - 7.533 \times 10^{-2}\ T + 1.842 \times 10^{-4}\ T^2 - 1.28 \times 10^{-7}\ T^3$	(38)
$CaSO_4 \cdot 2H_2O(s)$	400	$29.31 - 4.183 \times 10^{-2}\ T + 7.30 \times 10^{-5}\ T^2$	(38)

TABLE IV (CONTINUED)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
$Ca(NO_3)_2(s)$	800	$26.61 - 3.036 \times 10^{-2}\ T + 7.497 \times 10^{-5}\ T^2 - 3.77 \times 10^{-8}\ T^3$	(57)
$CaCO_3$ (calcite)	1000	$10.62 - 9.025 \times 10^{-3}\ T + 2.679 \times 10^{-5}\ T^2 - 1.221 \times 10^{-8}\ T^3$	(57)
Li(s)	454	$3.94 - 3.45 \times 10^{-3}\ T + 6.65 \times 10^{-6}\ T^2$	(10)
LiOH(s)	800	$6.35 - 1.06 \times 10^{-2}\ T + 2.60 \times 10^{-5}\ T^2 - 1.33 \times 10^{-8}\ T^3$	(9)
$LiOH \cdot H_2O(s)$	350	$8.61 + 5.1 \times 10^{-5}(T - 298.15)^2 - 1.6 \times 10^{-7}(T - 298.15)^3$	(57)
LiF(s)	1000	$4.55 - 4.06 \times 10^{-3}\ T + 1.25 \times 10^{-5}\ T^2 - 5.73 \times 10^{-9}\ T^3$	(9)
LiCl(s)	900	$7.67 - 6.29 \times 10^{-3}\ T + 1.73 \times 10^{-5}\ T^2 - 8.46 \times 10^{-9}\ T^3$	(9)
$Li_2SO_4(s)$	900	$15.53 - 1.863 \times 10^{-2}\ T + 4.831 \times 10^{-5}\ T^2 - 2.264 \times 10^{-8}\ T^3$	(9)
Na(s)	371	$6.17 + 1 \times 10^{-4}(T - 298.15) + 1.30 \times 10^{-5}(T - 298.15)^2$	(10)
NaOH(s)	600	$9.50 - 1.452 \times 10^{-2}\ T + 3.344 \times 10^{-5}\ T^2 - 1.619 \times 10^{-8}\ T^3$	(9)
NaF(s)	1000	$6.34 - 4.00 \times 10^{-3}\ T + 1.293 \times 10^{-5}\ T^2 - 6.03 \times 10^{-9}\ T^3$	(9)
NaCl(s)	1000	$8.83 - 4.09 \times 10^{-3}\ T + 1.346 \times 10^{-5}\ T^2 - 6.27 \times 10^{-9}\ T^3$	(9)
$Na_2S(s)$	1000	$11.81 - 6.48 \times 10^{-3}\ T + 2.167 \times 10^{-5}\ T^2 - 1.023 \times 10^{-8}\ T^3$	(9)
$Na_2SO_4(s)$	1000	$23.81 - 4.711 \times 10^{-2}\ T + 1.1182 \times 10^{-4}\ T^2 - 6.718 \times 10^{-8}\ T^3$	(9)
$Na_2SO_4 \cdot 10H_2O$	320	$71.15 + 3 \times 10^{-4}(T - 298.15)^2$	(57)

TABLE IV (CONTINUED)

Species	T_{max}, K	$-(G^o - H^o_{298})/RT =$	Ref.
$NaNO_3(s)$	550	$15.10 - 1.026 \times 10^{-2}\ T + 2.165 \times 10^{-5}\ T^2$	(57)
$Na_2CO_3(s)$	900	$18.15 - 1.809 \times 10^{-2}\ T + 4.595 \times 10^{-5}\ T^2 - 2.151 \times 10^{-8}\ T^3$	(9)
$NaHCO_3(s)$	400	$15.17 - 1.985 \times 10^{-2}\ T + 3.46 \times 10^{-5}\ T^2$	(57)
$NaCHO_2(s)$	330	$12.48 + 5 \times 10^{-5}(T - 298.15)^2$	(40)
$K(s)$	336	$7.78 + 2 \times 10^{-5}(T - 298.15)^2$	(10)
$KF(s)$	1000	$8.175 - 4.07 \times 10^{-3}\ T + 1.327 \times 10^{-5}\ T^2 - 6.185 \times 10^{-9}\ T^3$	(9)
$KCl(s)$	1000	$10.14 - 4.17 \times 10^{-3}\ T + 1.37 \times 10^{-5}\ T^2 - 6.377 \times 10^{-9}\ T^3$	(9)
$K_2SO_4(s)$	900	$22.88 - 1.898 \times 10^{-2}\ T + 5.042 \times 10^{-5}\ T^2 - 2.392 \times 10^{-8}\ T^3$	(9)
$K_2S_4O_6(s)$	330	$37.24 - 4 \times 10^{-4}(T - 298.15) + 1.7 \times 10^{-4}(T - 298.15)^2 - 5 \times 10^{-7}(T - 298.15)^3$	(37)
$KNO_3(s)$	400	$19.60 - 2.47 \times 10^{-2}\ T + 4.22 \times 10^{-5}\ T^2$	(57)

Appendix: Calculator Program for Use of Tables I-IV

For the reaction aA + bB = cC + dD, the constants of Table IV for each of the reactants and products can be combined to yield an equation for $-\Delta(G^o - H^o_{298})/RT$ as a function of temperature. The $\Delta H^o_{298}/R$ values of Tables I-III can be combined to yield $\Delta H^o_{298}/R$ for the overall reaction.

$$\Delta H^o_{298}/R = d(\Delta H^o_{298}/R)_D + c(\Delta H^o_{298}/R)_C - b(\Delta H^o_{298}/R)_B - a(\Delta H^o_{298}/R)_A$$

The equilibrium constant can then be calculated by the equation

$$\ln K_T = -\Delta(G^o - H^o_{298})/RT - (\Delta H^o_{298}/R)/T$$

If lnK is known, the above equation can be used to calculate $\Delta H^o_{298}/R$. The following program will carry out these operations using the constants of Tables I-IV. HP41C programing is used.

Directions:

		Display
(1) d ↑ c ↑ -b ↑ -a	XEQ 'AG'	0

The sign is negative for each reactant coefficient and positive for each product coefficient. If the total of reactants and products is three, enter d=0. For aA=cC, enter 0↑0↑c↑-a.

(2) $(a_0)_D$↑$(a_0)_C$↑$(a_0)_B$↑$(a_0)_A$	User A	$d(a_0)_D$
[(2') e STO9, $(a_0)_E$	User e	$e(a_0)_E$]

(2') is used only if the total of reactants and products is five. Step(2), and if necessary (2'), is repeated with a_1 values from Table IV, and then again with the a_2 values up to a_4 values if there are a_4 entries in Table IV for any of the reactants or products. If the sum of reactants and products is three, no entries are made for D. Similarly, if there are only two species, no entry is needed of $(a_n)_B$ values. If there are only a_0 terms which correspond to the C_p/R values at 298K given in Tables I-III, no entries are made after the a_0 entries. However, if any reactant or product has a higher term, then entries, even when they are zero, are required through the highest a_n set with at least one non-zero value.

(3a) T_1	XEQ 1	$-\Delta(G^o-H^o_{298})/RT_1$
(3b) (If I stored in R12)	R/S	$-\Delta(G^o-H^o_{298})/RT$ for $T=T_1+I$

(4) After 10.1 STO10, $\Delta H^o_{298}/R$ for each product and reactant is inserted as in (2), and if necessary (2').

(5a) To calculate average $\Delta H^o_{298}/R$ from a set of $\ln K_T$ values, XEQ 5 to set up registers

$T \uparrow \ln K_T$	User H	$\Delta H^o_{298}/R$
Repeat $T \uparrow \ln K$.H for all T.		
(5b)	R/S, SST	Av.$\Delta H^o_{298}/R$, Std.Dev.

(6a) After step 4 or 5 has stored $\Delta H^o_{298}/R$ in R11,

T_1	User E, SST	$\ln K_{T_1}$, K_{T_1}
(6b)	R/S, SST	$\ln K_T$, K_T for $T = T_1 + I$

Note 1: When $-(G^o - H^o_{298})/RT$ is given as a function of T-298.15, e.g. $a_0' + a_1'(T-298.15) + a_2(T-298.15)^2$, it is necessary to expand to obtain power series in T. In the example cited, $a_0 = a_0' - 298.15a_1' + a_2(298.15)^2$ and $a_1 = a_1' - 2(298.15)a_2$.

Note 2: When the $-(G^o - H^o_{298})/RT$ equation in Table IV contains lnT and T^{-1} terms, these terms should be entered by step (2) after insertion of the a_0 terms and before insertion of the a_1 terms. For an equation with lnT, T^{-1} as well as T and T^2 terms, LBL 01 would be modified after RCL 02 of step 51 to R↑ / + R↑ LN RCL 01 X + RCL 00 + RTN.

R 00	1	2	3	4	5	6	7	8	9	10
Δa_0	Δa_1	Δa_2	Δa_3	Δa_4	-a	-b	c	d	e	Δa Index

11	12	13	14	15	18
$\frac{\Delta H^o_{298}}{R}$	I	$\frac{\Sigma\Delta H^o_{298}}{R}$	$\Sigma\left(\frac{\Delta H^o_{298}}{R}\right)^2$	lnK	n

SIZE 019, program has 94 steps using 124 bytes or 18 registers or a total of 37 registers needed. Program will set Σ registers starting at 13.

Test:

$CaSO_3(s) = CaO(s) + SO_2(g)$

(1) 0 ↑ 1 ↑ 1 ↑ -1 XEQ 'AG' User

(2) 31.44 ↑ 4.82 ↑ 12.75 A

-1.4018×10^{-2}↑-4.07×10^{-3}↑ -9.16×10^{-3} A

3.8017×10^{-5}↑ 1.26×10^{-5}↑2.75×10^{-5} A

-3.37×10^{-8}↑-5.86×10^{-9}↑-1.236×10^{-8} A

1.0875×10^{-11} ↑ 0 ↑ 0 A

(3) EEX2 STO12, 800 XEQ1 21.694;

(3b) R/S 21.510; R/S 21.378

(4) 10.1 STO10, -35 700↑-76 380↑-139 400 A 0; RCL11 27 320

(6a) 800 E -12.456 SST 3.90×10^{-6}

(5a) XEQ5, 800↑ -12.46 H 27 324 900↑ -8.85 H 27 324

1000↑ -5.94 H 27 318 (5b) R/S 27 322, SST 3

```
PRP "AG"

 01♦LBL "AG"
STO 05  RDN  STO 06  RDN
STO 07  RDN  STO 08
-1.1  STO 10  0  STO 01
STO 02  STO 03  STO 04
STO 12  RTN

 18♦LBL A
ISG 10  STO IND 10  CLX
RCL 05  ST* IND 10  RDN
RCL 06  *  ST+ IND 10
RDN  RCL 07  *
ST+ IND 10  RDN  RCL 08
*  ST+ IND 10  RTN

 37♦LBL e
RCL 09  *  ST+ IND 10
RTN

 42♦LBL 01
ENTER↑  ENTER↑  ENTER↑
RCL 04  *  RCL 03  +  *
RCL 02  +  *  RCL 01  +
*  RCL 00  +  RTN
RCL 12  R↑  +  GTO 01

 64♦LBL 05
ΣREG 13  CLΣ  RTN

 68♦LBL H
STO 15  RDN  XEQ 01
RCL 15  -  R↑  *  Σ+
LASTX  RTN  MEAN  STO 11
RTN  SDEV

 83♦LBL E
XEQ 01  RCL 11  R↑  /  -
RTN  E↑X  RCL 12  R↑  +
GTO E  END
```

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