Thermodynamic Functions of the Gaseous Dioxides of Carbon, Nitrogen, Sulfur, and Chlorine, and of Carbon Disulfide and Oxysulfide

JOHN S. GORDON
Thiokol Chemical Corp., Denville, N. J.

AS DESCRIBED by Pennington and Kobe (*12*), thermodynamic properties of simple gaseous molecules may conveniently be described by the RRHO (rigid rotator–harmonic oscillator) approximation to which small correction terms are added to account for anharmonicities etc. Specific heat is affected the most, since it represents the second derivative of the state sum. An IBM 650 program was coded for triatomic gases using this method, as corrected by Woolley (*26*). He suggested that Pennington and Kobe's (*12*) Equation 23 should be corrected as follows:

$$C_e/R = 2sT + \sum_i d_i r_i \cdot {}^3\phi_i + \tfrac{1}{2} \sum_i d_i(d_i + 1)\, X_{ii} \cdot {}^6\phi_i + \sum_{i<j} d_i d_j X_{ij} \cdot {}^7\phi_i \cdot {}^7\phi_j \left[({}^8\phi_i + {}^8\phi_j)^2 + {}^9\phi_i + {}^9\phi_j - 1 \right]$$

This corrected C_e/R equation was used in the present calculations. It is assumed to give results equivalent to the calculation procedure set up by Woolley (*25*) for cases where α_{iii}, α_{iij}, α_{ijk}, y_{iii}, y_{iij}, and y_{ijk} are all zero, although we did not program his method as a check. Pennington and Kobe's Equation 23 is of course valid as originally stated for diatomic gases, and we have used it in deriving thermal data for over 80 diatomic gases (*6, 7*), but for triatomic gas it yields specific heat data which are inconsistent with enthalpy data. Replacement of ${}^{10}\phi$ by ${}^{9}\phi$ in their Equation 23 removes this inconsistency.

Molecular constants used in calculations are listed in Table I. Thermodynamic functions are listed in Tables II to VII, and apply to the ideal gaseous state at 1 atm. of partial pressure. The only thermodynamic data previously available for NO_2 and ClO_2 are based on the RRHO approximation, as is commonly done for polyatomic gases. Data for CS_2 and OCS have been compiled up to 1000° K. by Papousek (*11*). His results agree substantially with present work, although he used the RRHO approximation and obsolete vibrational frequencies for OCS (*g*).

T. Wentink (*23*) has noted that several of the internuclear distances for OCS and CS_2 tabulated by Papousek (*11*) are incorrect and are inconsistent with the references given by Papousek. These seem to be typographical errors, since Papousek's moments of inertia and thermodynamic functions agree substantially with present results.

RESULTS

For NO_2, three of the nine rotation-vibration interaction coefficients are given by Arakawa and Nielsen (*1*). The other six coefficients were taken as zero in these calculations, in the absence of specific data.

Table I. Molecular Constants

Species	CO_2	OCS	CS_2	NO_2	SO_2	ClO_2
ν_1, cm.$^{-1}$	1342.86	859	658	1319.7	1151.38	945.3
ν_2 [b]	667.3	524	396.8	749.8	517.69	447.4
ν_3	2349.16	2064	1532.5	1617.75	1361.76	1109
α_1, cm.$^{-1}$	0.00056	0.0006044	0.000156	$-0.0028 = \alpha_1^B$	0	0
α_2	−0.00062	−0.0003539	−0.000256	$0.36 = \alpha_2^A$	0	0
α_3	0.0029	0.001838	0.0007112	$-0.0024 = \alpha_3^B$	0	0
$-X_{11}$, cm.$^{-1}$	2.2	4.0	1.05	9.0	3.99	4.4
$-X_{22}$	0.75	0.4	−0.13	0.5	3.00	0
$-X_{33}$	12.5	7.0	5.14	16.4	5.17	2.0
$-X_{12}$	−3.76	6.8	−0.86	9.7	2.05	3.0
$-X_{23}$	11.58	11.5	6.67	2.7	3.90	13
$-X_{13}$	21.84	4.5	4.95	28.7	13.71	14.4
g_{22}, cm.$^{-1}$	1.03	3.2	0.67	0	0	0
A_{000}, cm.$^{-1}$	0	0	0	8.003	2.02773	1.6006
B_{000}	0.39026	0.20287	0.109099	0.434	0.344277	0.33283
C_{000}	0	0	0	0.412	0.293609	0.27553
D_{000}	1.26×10^{-7}	4.37×10^{-8}	1.2×10^{-8}	...	...	...
Mol. wt.	44.011	60.077	76.143	46.008	64.066	67.457
Symmetry no.	2	1	2	2	2	2
Stat. wt., g_0	1	1	1	2	1	2
Reference	(*10, 13, 19, 22*)	(*2, 3, 18, 20–22*)	(*9, 17*)	(*1*)	(*15, 16*)	(*4*)

[a] Observed fundamentals used in RRHO calculation.

[b] Double degeneracy when $A_0 = 0$ (linear molecule)

Table II. Thermodynamic Functions of NO_2 (g)

T, ° K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C_p°, Cal. Mole^{-1} Deg.$^{-1}$	$H^\circ - H^\circ_{298}$, Kcal. Mole^{-1}
298.15	49.174	8.1714	57.346	8.8566	
300	49.225	8.1557	57.401	8.8702	0.016397
400	51.612	8.4442	60.056	9.6352	0.94138
500	53.529	8.7578	62.287	10.377	1.9425
600	55.155	9.0832	64.238	11.024	3.0136
700	56.579	9.4002	65.979	11.561	4.1438
800	57.854	9.6986	67.553	11.997	5.3225
900	59.013	9.9742	68.987	12.349	6.5405
1000	60.077	10.226	70.303	12.634	7.7902
1100	61.062	10.456	71.519	12.868	9.0657
1200	61.981	10.665	72.647	13.062	10.362
1300	62.843	10.856	73.699	13.225	11.677
1400	63.654	11.030	74.685	13.363	13.006
1500	64.420	11.190	75.611	13.481	14.349
1600	65.147	11.336	76.484	13.584	15.702
1700	65.839	11.471	77.311	13.675	17.065
1800	66.498	11.596	78.095	13.755	18.437
1900	67.128	11.712	78.840	13.828	19.816
2000	67.732	11.819	79.551	13.893	21.202
2100	68.311	11.919	80.231	13.952	22.595
2200	68.867	12.013	80.881	14.007	23.993
2300	69.403	12.101	81.505	14.058	25.396
2400	69.920	12.183	82.104	14.105	26.804
2500	70.419	12.261	82.681	14.150	28.217
2600	70.902	12.335	83.237	14.192	29.634
2700	71.368	12.404	83.773	14.231	31.056
2800	71.821	12.470	84.291	14.269	32.481
2900	72.259	12.533	84.793	14.305	33.909
3000	72.685	12.592	85.278	14.340	35.342
3100	73.099	12.649	85.749	14.374	36.777
3200	73.502	12.704	86.206	14.406	38.216
3300	73.893	12.756	86.650	14.437	39.659
3400	74.275	12.806	87.081	14.468	41.104
3500	74.647	12.854	87.501	14.498	42.552
3600	75.010	12.900	87.910	14.527	44.004
3700	75.364	12.944	88.308	14.555	45.458
3800	75.709	12.987	88.697	14.583	46.915
3900	76.047	13.028	89.076	14.610	48.374
4000	76.378	13.068	89.446	14.637	49.837
4100	76.701	13.107	89.808	14.664	51.302
4200	77.017	13.144	90.162	14.690	52.770
4300	77.327	13.180	90.508	14.716	54.240
4400	77.630	13.215	90.846	14.741	55.713
4500	77.928	13.250	91.178	14.766	57.188
4600	78.219	13.283	91.503	14.791	58.666
4700	78.505	13.315	91.821	14.816	60.147
4800	78.786	13.347	92.133	14.840	61.630
4900	79.062	13.377	92.439	14.865	63.115
5000	79.332	13.407	92.740	14.889	64.603
5100	79.598	13.437	93.035	14.913	66.093
5200	79.859	13.465	93.325	14.936	67.585
5300	80.116	13.493	93.610	14.960	69.080
5400	80.368	13.521	93.889	14.983	70.577
5500	80.617	13.547	94.165	15.007	72.077
5600	80.861	13.574	94.435	14.030	73.579
5700	81.102	13.599	94.701	15.053	75.083
5800	81.338	13.625	94.964	15.076	76.590
5900	81.571	13.650	95.221	15.099	78.098
6000	81.801	13.674	95.475	15.122	79.609

Table III. Thermodynamic Functions of SO_2 (g)

T, ° K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C_p°, Cal. Mole^{-1} Deg.$^{-1}$
298.15	50.839	8.459	59.297	9.531
300	50.892	8.464	59.356	9.547
400	53.378	8.842	62.220	10.394
500	55.393	9.229	64.622	11.132
600	57.108	9.597	66.706	11.722
700	58.614	9.935	68.549	12.179
800	59.960	10.238	70.199	12.532
900	61.182	10.509	71.692	12.805
1000	62.302	10.750	73.053	13.021
1100	63.337	10.964	74.302	13.194
1200	64.300	11.156	75.456	13.334
1300	65.200	11.328	76.528	13.451
1400	66.045	11.484	77.529	13.548
1500	66.842	11.624	78.467	13.631
1600	67.596	11.752	79.349	13.703
1700	68.312	11.868	80.181	13.766
1800	68.994	11.975	80.970	13.822
1900	69.644	12.074	81.719	13.871
2000	70.266	12.165	82.431	13.916
2100	70.861	12.249	83.111	13.957
2200	71.433	12.328	83.761	13.995
2300	71.983	12.401	84.384	14.030
2400	72.512	12.470	84.982	14.062
2500	73.022	12.534	85.557	14.093
2600	73.515	12.594	86.110	14.121
2700	73.992	12.651	86.644	14.149
2800	74.453	12.705	87.159	14.175
2900	74.900	12.757	87.657	14.200
3000	75.333	12.805	88.138	14.224
3100	75.753	12.851	88.605	14.247
3200	76.162	12.895	89.058	14.269
3300	76.560	12.937	89.497	14.291
3400	76.946	12.977	89.924	14.312
3500	77.323	13.016	90.339	14.332
3600	77.690	13.053	90.743	14.353
3700	78.049	13.088	91.137	14.372
3800	78.398	13.122	91.521	14.392
3900	78.739	13.155	91.895	14.411
4000	79.073	13.186	92.260	14.429
4100	79.399	13.217	92.616	14.448
4200	79.718	13.246	92.965	14.466
4300	80.030	13.275	93.305	14.484
4400	80.335	13.303	93.638	14.502
4500	80.635	13.330	93.965	14.519
4600	80.928	13.356	94.284	14.537
4700	81.215	13.381	94.597	14.554
4800	81.497	13.406	94.903	14.571
4900	81.774	13.430	95.204	14.588
5000	82.045	13.453	95.499	14.605
5100	82.312	13.476	95.788	14.622
5200	82.574	13.498	96.072	14.638
5300	82.831	13.519	96.351	14.655
5400	83.084	13.541	96.625	14.671
5500	83.333	13.561	96.895	14.687
5600	83.577	13.582	97.160	14.704
5700	83.818	13.601	97.420	14.720
5800	84.055	13.621	97.676	14.736
5900	84.288	13.640	97.928	14.752
6000	84.517	13.659	98.176	14.768

Table IV. Thermodynamic Functions of CO_2 (g)

T, °K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C°_p, Cal. Mole^{-1} Deg.$^{-1}$	$H^\circ - H^\circ_{298}$, Kcal. Mole^{-1}
298.15	43.561	7.507	51.069	8.8724	
300	43.607	7.516	51.124	8.8926	0.016432
400	45.834	7.987	53.822	9.8732	0.95654
500	47.666	8.446	56.113	10.660	1.9846
600	49.244	8.870	58.115	11.305	3.0839
700	50.641	9.257	59.899	11.840	4.2420
800	51.901	9.609	61.510	12.286	5.4491
900	53.051	9.928	62.980	12.659	6.6970
1000	54.113	10.217	64.330	12.972	7.9790
1100	55.099	10.480	65.579	13.234	9.2898
1200	56.021	10.719	66.741	13.455	10.624
1300	56.888	10.937	67.825	13.643	11.979
1400	57.706	11.136	68.842	13.802	13.352
1500	58.481	11.318	69.799	13.939	14.739
1600	59.217	11.486	70.703	14.058	16.139
1700	59.918	11.640	71.558	14.160	17.550
1800	60.587	11.783	72.370	14.250	18.971
1900	61.228	11.915	73.143	14.330	20.400
2000	61.842	12.037	73.880	14.400	21.837
2100	62.432	12.151	74.584	14.462	23.280
2200	63.000	12.258	75.258	14.518	24.729
2300	63.547	12.357	75.905	14.569	26.183
2400	64.075	12.450	76.526	14.615	27.643
2500	64.585	12.538	77.123	14.656	29.106
2600	65.078	12.620	77.699	14.694	30.574
2700	65.556	12.697	78.254	14.729	32.045
2800	66.019	12.771	78.790	14.762	33.520
2900	66.469	12.840	79.309	14.792	34.998
3000	66.905	12.905	79.811	14.820	36.478
3100	67.329	12.967	80.297	14.846	37.961
3200	67.742	13.026	80.769	14.870	39.447
3300	68.144	13.083	81.227	14.893	40.936
3400	68.535	13.136	81.672	14.915	42.426
3500	68.917	13.187	82.104	14.935	43.919
3600	69.289	13.236	82.526	14.955	45.413
3700	69.652	13.283	82.936	14.974	46.910
3800	70.007	13.328	83.335	14.991	48.408
3900	70.354	13.371	83.725	15.008	49.908
4000	70.693	13.412	84.105	15.025	51.410
4100	71.024	13.451	84.476	15.040	52.913
4200	71.349	13.489	84.839	15.056	54.418
4300	71.667	13.526	85.193	15.070	55.924
4400	71.978	13.561	85.540	15.084	57.432
4500	72.283	13.595	85.879	15.098	58.941
4600	72.583	13.628	86.211	15.111	60.452
4700	72.876	13.660	86.536	15.124	61.964
4800	73.164	13.690	86.855	15.137	63.477
4900	73.447	13.720	87.167	15.149	64.991
5000	73.724	13.749	87.473	15.161	66.507
5100	73.997	13.776	87.774	15.173	68.023
5200	74.264	13.803	88.068	15.185	69.541
5300	74.528	13.830	88.358	15.196	71.060
5400	74.786	13.855	88.642	15.207	72.581
5500	75.041	13.880	88.921	15.218	74.102
5600	75.291	13.904	89.195	15.229	75.624
5700	75.537	13.927	89.465	15.239	77.148
5800	75.780	13.950	89.730	15.250	78.672
5900	76.018	13.972	89.991	15.260	80.198
6000	76.254	13.993	90.247	15.270	81.725

Table V. Thermodynamic Functions of ClO_2 (g)

T, °K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C°_p, Cal. Mole^{-1} Deg.$^{-1}$
298.15	52.795	8.657	61.453	10.037
300	52.849	8.665	61.515	10.057
400	55.406	9.137	64.544	11.010
500	57.495	9.588	67.083	11.743
600	59.279	9.994	69.274	12.278
700	60.848	10.250	71.198	12.668
800	62.250	10.659	72.909	12.957
900	63.522	10.927	74.449	13.175
1000	64.685	11.160	75.846	13.345
1100	65.759	11.365	77.125	13.480
1200	66.756	11.546	78.302	13.589
1300	67.686	11.707	79.394	13.680
1400	68.559	11.851	80.411	13.757
1500	69.382	11.980	81.362	13.824
1600	70.159	12.097	82.256	13.881
1700	70.895	12.204	83.099	13.933
1800	71.596	12.301	83.897	13.979
1900	72.263	12.390	84.654	14.020
2000	72.901	12.473	85.374	14.059
2100	73.511	12.549	86.061	14.094
2200	74.097	12.620	86.718	14.128
2300	74.659	12.687	87.346	14.159
2400	75.201	12.749	87.950	14.189
2500	75.722	12.807	88.529	14.217
2600	76.226	12.861	89.088	14.244
2700	76.712	12.913	89.626	14.270
2800	77.182	12.962	90.145	14.295
2900	77.638	13.008	90.647	14.319
3000	78.080	13.053	91.133	14.343
3100	78.509	13.095	91.604	14.366
3200	78.925	13.135	92.060	14.389
3300	79.330	13.173	92.503	14.411
3400	79.724	13.210	92.934	14.433
3500	80.107	13.245	93.352	14.454
3600	80.481	13.279	93.760	14.475
3700	80.845	13.311	94.157	14.496
3800	81.200	13.343	94.544	14.516
3900	81.547	13.373	94.921	14.537
4000	81.886	13.403	95.289	14.557
4100	82.218	13.431	95.649	14.576
4200	82.542	13.458	96.001	14.596
4300	82.859	13.485	96.344	14.616
4400	83.169	13.511	96.681	14.635
4500	83.473	13.536	97.010	14.654
4600	83.771	13.561	97.332	14.674
4700	84.063	13.585	97.648	14.693
4800	84.349	13.608	97.957	14.712
4900	84.630	13.631	98.261	14.730
5000	84.905	13.653	98.559	14.749
5100	85.176	13.674	98.851	14.768
5200	85.442	13.696	99.138	14.787
5300	85.703	13.716	99.420	14.805
5400	85.959	13.737	99.697	14.824
5500	86.212	13.757	99.969	14.842
5600	86.460	13.776	100.236	14.860
5700	86.704	13.795	100.500	14.879
5800	86.944	13.814	100.759	14.897
5900	87.180	13.833	101.013	14.915
6000	87.413	13.851	101.264	14.934

Table VI. Thermodynamic Functions of CS_2 (g)

T, ° K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C_p°, Cal. Mole^{-1} Deg.$^{-1}$	$H^\circ - H^\circ_{298}$, Kcal. Mole^{-1}
298.15	48.281	8.5502	56.831	10.874	
300	48.334	8.5646	56.898	10.895	0.020136
400	50.898	9.2702	60.168	11.820	1.1588
500	53.030	9.8495	62.880	12.480	2.3754
600	54.870	10.331	65.201	12.973	3.5493
700	56.494	10.736	67.231	13.348	4.9663
800	57.951	11.081	69.033	13.635	6.3161
900	59.274	11.378	70.652	13.858	7.6913
1000	60.486	11.635	72.121	14.032	9.0861
1100	61.606	11.859	73.466	14.171	10.496
1200	62.646	12.057	74.704	14.283	11.919
1300	63.619	12.232	75.851	14.374	13.352
1400	64.531	12.388	76.919	14.450	14.794
1500	65.390	12.527	77.918	14.513	16.242
1600	66.203	12.653	78.857	14.566	17.696
1700	66.974	12.767	79.741	14.612	19.155
1800	67.706	12.871	80.577	14.651	20.618
1900	68.405	12.965	81.371	14.686	22.085
2000	69.072	13.052	82.125	14.716	23.555
2100	69.711	13.132	82.843	14.742	25.028
2200	70.324	13.206	83.530	14.766	26.504
2300	70.912	13.274	84.187	14.787	27.981
2400	71.478	13.337	84.816	14.806	29.461
2500	72.024	13.396	85.421	14.823	30.943
2600	72.551	13.452	86.003	14.839	32.426
2700	73.059	13.503	86.563	14.854	33.911
2800	73.551	13.552	87.104	14.867	35.397
2900	74.028	13.579	87.625	14.880	36.884
3000	74.489	13.640	88.130	14.891	38.373
3100	74.937	13.681	88.619	14.902	39.862
3200	75.372	13.719	89.092	14.912	41.353
3300	75.795	13.755	89.551	14.922	42.845
3400	76.206	13.790	89.997	14.931	44.338
3500	76.606	13.823	90.430	14.940	45.831
3600	76.996	13.854	90.851	14.948	47.326
3700	77.376	13.883	91.260	14.956	48.821
3800	77.747	13.912	91.659	14.963	50.317
3900	78.109	13.939	92.048	14.970	51.813
4000	78.462	13.965	92.427	14.977	53.311
4100	78.807	13.989	92.797	14.984	54.809
4200	79.144	14.013	93.158	14.990	56.308
4300	79.474	14.036	93.511	14.997	57.807
4400	79.797	14.058	93.856	15.003	59.307
4500	80.114	14.079	94.193	15.009	60.808
4600	80.423	14.099	94.523	15.014	62.309
4700	80.727	14.119	94.846	15.020	63.811
4800	81.024	14.138	95.162	15.026	65.313
4900	81.316	14.156	95.472	15.031	66.816
5000	81.602	14.173	95.776	15.036	68.319
5100	81.883	14.190	96.074	15.041	69.823
5200	82.159	14.207	96.366	15.046	71.328
5300	82.429	14.223	96.652	15.051	72.833
5400	82.695	14.238	96.934	15.056	74.338
5500	82.957	14.253	97.210	15.061	75.844
5600	83.214	14.267	97.482	15.066	77.351
5700	83.466	14.281	97.748	15.071	78.857
5800	83.715	14.295	98.010	15.075	80.365
5900	83.959	14.308	98.268	15.080	81.873
6000	84.200	14.321	98.522	15.084	83.381

Table VII. Thermodynamic Functions of OCS (g)

T, ° K.	$-(F^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C_p°, Cal. Mole^{-1} Deg.$^{-1}$
298.15	47.363	7.959	55.323	9.917
300	47.413	7.971	55.384	9.940
400	51.773	9.147	60.920	10.958
500	51.773	9.147	60.920	11.687
600	53.483	9.619	63.103	12.249
700	54.998	10.028	65.026	12.700
800	56.361	10.386	66.747	13.067
900	57.602	10.701	68.304	13.370
1000	58.745	10.981	69.726	13.620
1100	59.803	11.231	71.034	13.829
1200	60.790	11.455	72.245	14.004
1300	61.715	11.657	73.372	14.153
1400	62.586	11.840	74.426	14.280
1500	63.409	12.006	75.415	14.389
1600	64.188	12.158	76.347	14.485
1700	64.930	12.297	77.228	14.569
1800	65.636	12.426	78.062	14.643
1900	66.311	12.544	78.856	14.709
2000	66.958	12.654	79.612	14.769
2100	67.578	12.756	80.334	14.824
2200	68.173	12.851	81.025	14.873
2300	68.747	12.940	81.687	14.919
2400	69.299	13.023	82.323	14.962
2500	69.832	13.102	82.935	15.001
2600	70.348	13.175	83.524	15.038
2700	70.846	13.245	84.092	15.073
2800	71.329	13.311	84.641	15.106
2900	71.797	13.373	85.171	15.137
3000	72.252	13.433	85.685	15.167
3100	72.693	13.489	86.183	15.195
3200	73.122	13.543	86.666	15.223
3300	73.540	13.594	87.134	15.249
3400	73.946	13.643	87.590	15.275
3500	74.343	13.690	88.033	15.299
3600	74.729	13.735	88.465	15.323
3700	75.106	13.778	88.885	15.347
3800	75.474	13.820	89.294	15.370
3900	75.833	13.860	89.694	15.392
4000	76.185	13.899	90.084	15.414
4100	76.528	13.936	90.465	15.435
4200	76.865	13.972	90.837	15.456
4300	77.194	14.007	91.201	15.477
4400	77.516	14.040	91.557	15.497
4500	77.832	14.073	91.905	15.517
4600	78.142	14.104	92.247	15.537
4700	78.446	14.135	92.581	15.556
4800	78.743	14.165	92.909	15.576
4900	79.036	14.194	93.230	15.595
5000	79.323	14.222	93.545	15.614
5100	79.605	14.250	93.855	15.632
5200	79.882	14.276	94.159	15.651
5300	80.154	14.302	94.457	15.669
5400	80.422	14.328	94.750	15.687
5500	80.685	14.353	95.038	15.705
5600	80.944	14.377	95.321	15.723
5700	81.198	14.401	95.600	15.741
5800	81.449	14.424	95.874	15.759
5900	81.696	14.447	96.143	15.777
6000	81.939	14.469	96.408	15.794

For SO_2, none of the α_i have been reported, and all are taken as zero in these calculations. The anharmonic coefficients were reported by Shelton, Nielsen, and Fletcher (*15*) after publication by Evans and Wagman (*5*) of thermodynamic functions based on estimated anharmonicity coefficients. Their estimates were excellent in that the C_p^0 difference at 1500° K. is only 0.13%.

For CO_2, the specific heat at 5000° K. is 0.9% lower than given in the tabulation by Woolley (*24*). This is attributed to the recently revised X_{21} and D_{000} used here, plus the absence of a Fermi resonance correction term in our calculation method.

For ClO_2, no α_i have been reported, and all are taken as zero in these calculations. The statistical weight of the ground state was taken as 2, since this is an odd molecule. The National Bureau of Standards RRHO tables (*14*) appear to omit this multiplicity. However, the possibility remains that $g_0 = 4$ ($^2\pi$ ground state) by analogy with Cl and ClO.

For CS_2, the set of anharmonicities derived by Wentink (*22*) from the infrared data of Guenther, Wiggins, and Rank (*9*) lead to negative corrections of thermodynamic functions, due to the high values of g_{22} and X_{12}. Following the recommendations of Wentink (*22*), the set of anharmonicities reported by Stoichieff (*17*) was used in these calculations, and the usual positive corrections for C_p were obtained.

The present table for OCS duplicates unpublished calculations by Sanford Gordon (*8*). Values of D_i differ by 22% between those given in (*2*) and (*18*).

Estimated thermodynamic data for related molecules such as PO_2, SiO_2, and TiO_2 were published recently (*7*). Data for H_2S, FCN, ClCN, and BrCN have been calculated and will be published subsequently.

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