0 to 6000 K Ideal Monatomic Gas

IP(Xe, g) = 97834.0 ± 0.1 cm^{-1}
$S°(298.15\ K) = 169.684 \pm 0.003\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = 0\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1S_0$	0	1

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

Information on the electronic energy levels and quantum weights is taken from Moore.[1,9] Many of the theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[2] has no effect on the thermodynamic properties to 6000 K. This is undoubtedly a result of the high energy of these levels; the first excited level is over 67000 cm^{-1} above the ground state. Therefore, we list the ground state only. Extension to higher temperatures may require consideration of excited states and utilization of different fill and cutoff procedures.[2]

The thermodynamic functions at 298.15 K agree exactly with recent CODATA recommendations[3] except for two minor changes. First, the entropy differs by 0.1094 $J\cdot K^{-1}\cdot mol^{-1}$ because this table uses a reference pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, entropy differences of the order of 0.001–0.004 $J\cdot K^{-1}\cdot mol^{-1}$ for the rare gases arise due to the use of slightly different values for R and the relative atomic mass; this table uses R = 8.31441 $J\cdot K^{-1}\cdot mol^{-1}$. Within these same minor changes, the tables agree within the estimated uncertainty with those by Hultgren *et al.*,[4] Hilsenrath *et al.*,[5] Gurvich *et al.*,[8] and Wagman *et al.*[12] The estimated uncertainty is due to uncertainties in the relative atomic mass and fundamental constants which are based on the 1981 scale[6] and the 1973 values[7], respectively.

Phase Data

The triple point, 161.388 K, and boiling point, 165.060 K, are secondary fixed points of IPTS–68.[10,11] Hultgren *et al.*[4] had recommended a triple point of 161.36 K (0.8059 atm) and a boiling point of 165.060 K (1 atm). These values are provided for the convenience of the reader and have not been evaluated by the present authors. As a result of the low values, the reference state for xenon is chosen to be the ideal gas at all temperatures. This may differ from the choice of other authors.

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Enthalpy Reference Temperature = T_r = 298.15 K; Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-6.197	0.	0.	0.
100	20.786	146.977	188.164	-4.119	0.	0.	0.
200	20.786	161.384	171.585	-2.040	0.	0.	0.
250	20.786	166.023	170.026	-1.001	0.	0.	0.
298.15	20.786	169.684	169.684	0.	0.	0.	0.
300	20.786	169.812	169.684	0.038	0.	0.	0.
350	20.786	173.017	169.937	1.078	0.	0.	0.
400	20.786	175.792	170.499	2.117	0.	0.	0.
450	20.786	178.240	171.226	3.156	0.	0.	0.
500	20.786	180.430	172.039	4.196	0.	0.	0.
600	20.786	184.220	173.763	6.274	0.	0.	0.
700	20.786	187.424	175.492	8.353	0.	0.	0.
800	20.786	190.200	177.161	10.431	0.	0.	0.
900	20.786	192.648	178.748	12.510	0.	0.	0.
1000	20.786	194.838	180.249	14.589	0.	0.	0.
1100	20.786	196.819	181.667	16.667	0.	0.	0.
1200	20.786	198.628	183.006	18.746	0.	0.	0.
1300	20.786	200.292	184.273	20.824	0.	0.	0.
1400	20.786	201.832	185.473	22.903	0.	0.	0.
1500	20.786	203.266	186.612	24.982	0.	0.	0.
1600	20.786	204.608	187.695	27.060	0.	0.	0.
1700	20.786	205.868	188.727	29.139	0.	0.	0.
1800	20.786	207.056	189.713	31.217	0.	0.	0.
1900	20.786	208.180	190.655	33.296	0.	0.	0.
2000	20.786	209.246	191.559	35.375	0.	0.	0.
2100	20.786	210.260	192.425	37.453	0.	0.	0.
2200	20.786	211.227	193.258	39.532	0.	0.	0.
2300	20.786	212.151	194.059	41.610	0.	0.	0.
2400	20.786	213.036	194.832	43.689	0.	0.	0.
2500	20.786	213.884	195.577	45.768	0.	0.	0.
2600	20.786	214.699	196.297	47.846	0.	0.	0.
2700	20.786	215.484	196.993	49.925	0.	0.	0.
2800	20.786	216.240	197.667	52.004	0.	0.	0.
2900	20.786	216.969	198.320	54.082	0.	0.	0.
3000	20.786	217.674	198.954	56.161	0.	0.	0.
3100	20.786	218.355	199.569	58.239	0.	0.	0.
3200	20.786	219.015	200.166	60.318	0.	0.	0.
3300	20.786	219.655	200.747	62.397	0.	0.	0.
3400	20.786	220.276	201.312	64.475	0.	0.	0.
3500	20.786	220.878	201.863	66.554	0.	0.	0.
3600	20.786	221.464	202.399	68.632	0.	0.	0.
3700	20.786	222.033	202.922	70.711	0.	0.	0.
3800	20.786	222.587	203.432	72.790	0.	0.	0.
3900	20.786	223.127	203.930	74.868	0.	0.	0.
4000	20.786	223.654	204.417	76.947	0.	0.	0.
4100	20.786	224.167	204.892	79.025	0.	0.	0.
4200	20.786	224.668	205.357	81.104	0.	0.	0.
4300	20.786	225.157	205.812	83.183	0.	0.	0.
4400	20.786	225.635	206.257	85.261	0.	0.	0.
4500	20.786	226.102	206.693	87.340	0.	0.	0.
4600	20.786	226.559	207.120	89.418	0.	0.	0.
4700	20.786	227.006	207.538	91.497	0.	0.	0.
4800	20.786	227.443	207.949	93.576	0.	0.	0.
4900	20.786	227.872	208.351	95.654	0.	0.	0.
5000	20.786	228.292	208.745	97.733	0.	0.	0.
5100	20.786	228.704	209.133	99.811	0.	0.	0.
5200	20.786	229.107	209.513	101.890	0.	0.	0.
5300	20.786	229.503	209.886	103.969	0.	0.	0.
5400	20.786	229.892	210.253	106.047	0.	0.	0.
5500	20.786	230.273	210.614	108.126	0.	0.	0.
5600	20.786	230.648	210.968	110.204	0.	0.	0.
5700	20.786	231.015	211.317	112.283	0.	0.	0.
5800	20.786	231.377	211.659	114.362	0.	0.	0.
5900	20.786	231.732	211.997	116.440	0.	0.	0.
6000	20.786	232.082	212.329	118.519	0.	0.	0.

PREVIOUS: March 1977 (1 atm) CURRENT: March 1982 (1 bar)

IP(Xe^+, g) = 171068.4 ± 0.2 cm^{-1}
$S°$(298.15 K) = 181.210 ± 0.003 $J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°$(0 K) = 1170.355 ± 0.001 $kJ \cdot mol^{-1}$
$\Delta_f H°$(298.15 K) = [1176.552] $kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^2P_{3/2}$	0	4
$^2P_{1/2}$	10537.01	2

Enthalpy of Formation

The ionization limit of neutral xenon (97834 0 ± 0 1 cm^{-1}) reported by Moore[1] is adopted as $\Delta_f H°$(0 K) for Xe^+(g). The ionization limit is converted from cm^{-1} to $kJ \cdot mol^{-1}$ using the factor, 1 cm^{-1} = 0.01196266 $kJ \cdot mol^{-1}$, which is derived from the latest CODATA fundamental constants.[2] The uncertainty in the ionization limit is estimated to be ±0.1 cm^{-1} which corresponds to an uncertainty of ±0.001 $kJ \cdot mol^{-1}$ in the heat of formation. Rosenstock *et al.*[9] and Levine and Lias[11] have summarized additional ionization potential and appearance potential data. Gurvich *et al.*[8] and Wagman *et al.*[10] adopted the same ionization potential, but the use of slightly different fundamental constants by Wagman *et al.*[10] results in a heat of formation difference of 0.011 $kJ \cdot mol^{-1}$.

$\Delta_f H°$(Xe^+, g, 298.15 K) is obtained from $\Delta_f H°$(Xe, g, 0 K) by using IP(Xe) with JANAF[3] enthalpies $H°(0\ K)-H°(298.15\ K)$ for Xe^+(g), Xe(r), and e^-(r). $\Delta_r H°$($Xe \rightarrow Xe^+ + e^-$, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[9] $\Delta_f H°$(298.15 K) should be changed by −6.197 $kJ \cdot mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights of Moore[4] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[5] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the $^2P_{1/2}$ level, the next lowest level is over 90000 cm^{-1} above the ground state. Since inclusion of these upper levels has no effect on the thermodynamic functions (to 6000 K) we list only the ground state and the $^2P_{1/2}$ state, with the energy of the latter state taken from a more recent study by Moore.[1] The reported uncertainty in $S°$(298.15 K) is due to uncertainties in the relative ionic mass and fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states and use of different fill and cutoff procedures.[5]

The thermodynamic functions reported here agree with those of Green *et al.*,[6] Hilsenrath *et al.*,[7] and Gurvich *et al.*[8] except for two minor changes. First, the entropy differs by 0.1094 $J \cdot K^{-1} \cdot mol^{-1}$ because this table uses a standard state pressure of 1 bar, whereas the cited references used a pressure of 1 atm. Second, smaller differences arise from the use of different values for the fundamental constants, the relative ionic mass, and the position of the $^2P_{1/2}$ electronic level.

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Enthalpy Reference Temperature = T_r = 298.15 K; Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.197	1170.355		
100	20.786	158.503	199.690	−4.119			
200	20.786	172.910	183.111	−2.040			
250	20.786	177.549	181.552	−1.001			
298.15	20.786	181.210	181.210	0.	1176.552	1166.861	−204.429
300	20.786	181.338	181.210	0.038	1176.591	1166.801	−203.158
350	20.786	184.543	181.463	1.078	1177.630	1165.087	−173.880
400	20.786	187.318	182.026	2.117	1178.669	1163.224	−151.902
450	20.786	189.766	182.752	3.156	1179.709	1161.231	−134.792
500	20.786	191.957	183.565	4.196	1180.748	1159.123	−121.093
600	20.786	195.746	185.289	6.274	1182.826	1154.602	−100.517
700	20.786	198.950	187.018	8.353	1184.905	1149.734	−85.794
800	20.786	201.726	188.687	10.431	1186.984	1144.568	−74.733
900	20.786	204.174	190.274	12.510	1189.062	1139.141	−66.114
1000	20.786	206.364	191.776	14.589	1191.141	1133.483	−59.207
1100	20.787	208.345	193.193	16.667	1193.220	1127.616	−53.546
1200	20.788	210.154	194.532	18.746	1195.298	1121.561	−48.820
1300	20.791	211.818	195.799	20.825	1197.377	1115.331	−44.815
1400	20.796	213.359	196.999	22.904	1199.457	1108.942	−41.375
1500	20.803	214.794	198.138	24.984	1201.536	1102.404	−38.389
1600	20.815	216.137	199.221	27.065	1203.617	1095.728	−35.772
1700	20.830	217.399	200.254	29.147	1205.700	1088.921	−33.458
1800	20.851	218.591	201.240	31.231	1207.784	1081.991	−31.399
1900	20.877	219.719	202.183	33.318	1209.870	1074.946	−29.552
2000	20.908	220.790	203.087	35.407	1211.959	1067.791	−27.888
2100	20.945	221.811	203.954	37.499	1214.052	1060.531	−26.379
2200	20.987	222.787	204.788	39.596	1216.148	1053.171	−25.005
2300	21.033	223.720	205.591	41.697	1218.249	1045.716	−23.749
2400	21.085	224.617	206.366	43.803	1220.355	1038.170	−22.595
2500	21.141	225.479	207.113	45.914	1222.466	1030.535	−21.532
2600	21.200	226.309	207.835	48.031	1224.583	1022.816	−20.549
2700	21.262	227.110	208.534	50.154	1226.706	1015.016	−19.637
2800	21.326	227.884	209.212	52.283	1228.836	1007.136	−18.788
2900	21.392	228.634	209.869	54.419	1230.972	999.181	−17.997
3000	21.460	229.360	210.506	56.562	1233.114	991.152	−17.257
3100	21.528	230.065	211.126	58.711	1235.264	983.051	−16.564
3200	21.596	230.750	211.729	60.868	1237.420	974.880	−15.913
3300	21.664	231.415	212.315	63.031	1239.583	966.643	−15.301
3400	21.732	232.063	212.886	65.200	1241.753	958.339	−14.723
3500	21.798	232.694	213.443	67.377	1243.929	949.972	−14.178
3600	21.863	233.309	213.987	69.560	1246.112	941.542	−13.661
3700	21.927	233.909	214.517	71.749	1248.302	933.052	−13.172
3800	21.988	234.494	215.035	73.945	1250.497	924.502	−12.708
3900	22.048	235.066	215.541	76.147	1252.699	915.895	−12.267
4000	22.105	235.625	216.037	78.355	1254.907	907.230	−11.847
4100	22.160	236.172	216.521	80.568	1257.120	898.511	−11.447
4200	22.213	236.706	216.995	82.787	1259.339	889.738	−11.066
4300	22.263	237.230	217.460	85.011	1261.563	880.911	−10.701
4400	22.311	237.742	217.915	87.239	1263.791	872.033	−10.352
4500	22.356	238.244	218.361	89.473	1266.025	863.105	−10.019
4600	22.398	238.736	218.799	91.710	1268.263	854.126	−9.699
4700	22.438	239.218	219.228	93.952	1270.504	845.099	−9.392
4800	22.476	239.691	219.649	96.198	1272.750	836.024	−9.098
4900	22.511	240.154	220.063	98.447	1274.999	826.902	−8.815
5000	22.543	240.610	220.470	100.700	1277.252	817.735	−8.543
5100	22.573	241.056	220.869	102.956	1279.508	808.522	−8.281
5200	22.601	241.495	221.261	105.214	1281.767	799.265	−8.029
5300	22.626	241.926	221.647	107.476	1284.028	789.964	−7.786
5400	22.650	242.349	222.027	109.740	1286.292	780.621	−7.551
5500	22.671	242.765	222.400	112.006	1288.558	771.236	−7.325
5600	22.690	243.173	222.767	114.274	1290.826	761.810	−7.106
5700	22.707	243.575	223.129	116.544	1293.096	752.343	−6.894
5800	22.722	243.970	223.485	118.815	1295.367	742.836	−6.690
5900	22.736	244.359	223.835	121.088	1297.640	733.290	−6.492
6000	22.747	244.741	224.180	123.362	1299.914	723.706	−6.300

PREVIOUS: March 1977 (1 atm) CURRENT: March 1982 (1 bar)