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Refer to the individual tables for details

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Standard State Pressure = p = 0.1 MPa

J. mol ΔH

 $H^{\bullet}-H^{\circ}(T_{\epsilon})$

log K

CRYSTAL(a)

 $S'(298.15 \text{ K}) = 38.87 \pm 0.2 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$

Zirconium, Alpha (α–Zr)

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Enthalpy Reference Temperature = T, = 298.15 K $S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{\bullet})]T$ L.K-100-1 ئ

 $\Delta_p H^{\circ}(0 \text{ K}) = 0 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = 0 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_{\rm cr}H^{\circ} = 4.017 \pm 0.3 \text{ kJ} \cdot \text{mol}^{-1}$

0. 14.055 29.050 34.474 38.869 39.025 42.943 46.384 49.457

0. 18.617 24.693 25.202

25.218 25.935 25.935 26.246 26.564

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Todd, ³ and Scott. ⁶ The mathematical and graphical treatment of these four studies yields a continuous and smooth heat capacity curve. There are six studies^{1,22-10} on the heat capacity of zirconium in the region 1–5 K. Only Wolcott² reported the experimental data (60 data

The adopted thermal functions for α-Zr(cr) are derived from the studies of Collings and Ho, Wolcott, Burk et al., 3 Skinner and Johnston,

Heat Capacity and Entropy

Enthalpy of Formation r... = 1135 ± 10 K (α-β)

Zero by definition.

J. Phys. Chem. Ref. Data, Monograph 9

soints). In the other studies, an equation (with two constants) was given to describe the entire set of experimental data. The constants given cal-mol⁻¹ K^{-1} , with the adopted value being S'(5K) = 0.0043 cal-mol⁻¹ K^{-1} Similarly for $C_p'(5K)$ the maximum difference is 0.00073 cal-mol⁻¹ K^{-1} , with the adopted value being $C_p'(5K) = 0.00610$ cal-mol⁻¹ K^{-1} In the region above 5 K and below 300 K, there are four heat capacity studies. 25 There is much scatter among the different studies, between 150 and 300 K. From 150-200 K, we adopt graphically smoothed C, values internediate between Burk et al., 2 Skinner and Johnston, 4 and Todd 5 From 200-300 K, we adopt the data of Skinner and Johnston, 4 because it meshes better with the high temperature data. Burk's data

by Collings and Ho and the data of Wolcott* were used in this region. The maximum difference in the calculated values for S°(5 K) is 0.00029

27.281 28.053 28.966 30.003 31.128 32,306

32.724

75.939

23.851 26.004 29.413 32.938 36.572 40.304 44.119

-3.170 -2.556 -1.886

0.010 -0.021 -0.035 -0.038 -0.040

0.222 0.528 0.790 1.006 1.176

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38.869 38.870 39.178 39.868 40.756 41.776

0.047 1.318 2.606 3.911 5.231

7.922 10.689 13.538 16.486 19.542 22.713

45.939 46.136 48.287 50.363 52.357 54.272

54.925

56.113 57.886 59.596 61.249 62.848 64.398

57.143 61.406 65.210 68.680 71.899

is 1.4% higher than the adopted at 170 K, Todd's data is 0.7% higher and Skinner's data is 1% lower. Todd's data is 3% higher than the

Between 300 K and 1135 K there are three heat capacity studies^{6 II I2} and seven enthalpy studies. ¹³⁻¹⁹ The three heat capacity studies show

actually used in the fit. None of Scott's data below 540 K were used in the fit, becuase the data had a hump in this region and appeared to

much scatter and disagreement. The data of Scott⁶ was adopted, although only the data from runs 17 and 64, out of a total of nine runs, was

adopted at 300 K.

be high. The region between the low temperature data (300 K) and 540 K was graphically smoothed to assure continuity in the C, curve. The data of Scott⁵ is about 5% higher than the adopted between 300 and 540 K. Between 540 and 960 K it is within ±3% of the adopted, From

960 K to the transition temperature, there is much scatter; some of the data are as much as 20% higher than the adopted. The data of Vollmer et al. i are about 3% lower than the adopted at 300 K. Between 540 and 580 it agrees with the adopted. From 580-1000 K it is about 1.5%

Transition Data

higher than the adopted. The data of Klein and Danielson¹¹ was given only as a graph. It is considerably lower than the adopted values. The enthalpy studies show an unusually large scatter within each study, as well as a lack of agreement between the studies. When plotted as mean heat capacity, the seven studies are all higher than the adopted values, by 2 to 40%.

Refer to the β-Zr(cr) table for details.

There are no experimental sublimation studies involving α -Zr(cr) The enthalpy of sublimation is calculated as the difference between the Sublimation Data

enthalpy of formation of the monatomic gas and the enthalpy of formation of α -Zr(cr).

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CURRENT: June 1979

Zirconium, Alpha (Zr)

PREVIOUS. December 1967

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Zr₁(cr)

Zirconium, Beta (Zr)

PREVIOUS: December 1967

Ar = 91.22 Zirconium, Beta (Zr)

Zr₁(cr)

CRYSTAL(B) S°(298.15 K) = [43.192] J·K⁻¹·mol⁻¹ Zirconium, Beta (B-Zr) trs = 1135 ± 10 K (α - β)

f_{tot} = 2125 ± 15 K (β-1)

The enthalpy of formation is calculated from that of the a-crystal by addition of \$\Delta_{\mu}H^*\$ and the difference in enthalpy, \$H^(1)\$ H°(298.15 K), between the α-crystal and the β-crystal. **Enthalpy of Formation**

Heat Capacity and Entropy

were 5-10% lower than the adopted. The enthalpy studies show an unusually large scatter within each study, as well as lack of agr between the studies. Like the α-Ζτ(στ), the mean heat capacities are all higher than the adopted values, by 3 to 10%. The entropy at 25 There are five heat capacity studies 1-3 and five enthalpy studies 6-10 over the temperature range 1135-2125 K. The adopted values were adopted. The data of Rumyantsu et al. 3 were largely scattered and about 15% high. The data of Vollmer et al.? and of Klein and Dar on the heat capcity study of Cezairliyan and Righini. The data of Scott showed much scatter with a maximum deviation of 7% f is calculated in a manner similar to that for the enthalpy of formation.

Phase Data

Zirconium, at ambient pressures, exists in two crystal modifications. The low temperature form, α-Zr, is hexagonal close packed, (A3) structure isotypic with Mg. The high temperature form, \(\beta\)-Zt, is body centered cubic, a bcc (A2) structure

The transition temperature and enthalpies of transition are summarized in the table below. The adopted value of T_{rn} is 1135 ± 10 adopted $\Delta_{ur}H^{\circ}$ is 4.017 kJ·mol⁻

Source	T _{to} /K	Δ _{tr} H°, kcal·mol ⁻¹	Purity	Method
Vogel and Tonn ¹¹	1135 ± 5			cooling and dilatometric curves
laeger and Veenstra12	<1150	•	1	drop calorimetry
Coughlin and King ⁶	1135	0.920	97.85	drop calorimetry
Dewey ¹³	1138 ± 10	t		cooline curve
Skinner7	1143 ± 5	1.042	99.05	dron calorimetry
Komar and Shrednik ¹⁴	1135	.	1	election microscope
Scott'	1143 ± 2	0.993 ± 0.025	ı	adiabatic calorimetry
Douglas and Victor	1136	0.894	16.66	drop calorimetry
Sertzricken and Slyusar15	1135	0.712 ± 0.060		differential calorimetry
Klein and Danielson ²	1138		1	resistivity
Rudy et al. 16	1145 ± 15	1	99.81	differential thermal analysis
/ollmer et al.3	1155	0.950	866	adiabatic calorimetry
eletskii et al. 17	1148 ± 5	,	} 1	resistivity
Martynyuk and Tsapkov18	1	1.076	97.66	resistivity

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The sublimation studies involving \(\beta\)-\(\frac{Zt}{ct}\) are summarized on the \(\frac{Zt}{c}\) table. The enthalpy of sublimation for \(\beta\)-\(\frac{Zt}{ct}\) is calcul the difference in the enthalpies of formation at 298.15 K of Zr(g) and β-Zr(cr).

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Continued on page 1951

$\Delta_{\rm tr} T (296.13 \text{ K}) = [4.810] \text{ KJ-mol}^{-1}$	rumanpy r	elerence 1	J·K-'mol-'	randally reference temperature = I, = 298.15 K		Standard State Pressure = $p^* = 0.1 \text{ MPa}$ k1·mol ⁻¹	Pressure = p	- 0.1 MPa
$\Delta_{\text{fug}}H^{\circ} = 20.92 \pm 6.3 \text{ kJ} \cdot \text{mol}^{-1}$	τÆ	ಚ	S -[G	$S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{\bullet})]T$	$H^{\bullet}-H^{\bullet}(T_{r})$	Δ,Η*	Δ _C	log Kr
difference in enthalpy, H°(1135 K)-	°8888							
25 K. The adopted values were based	298 15 300 350	25.202 25.218 25.587	43.192 43.348 47.264	43.192	0.0047	4.810 4.809	3.521 3.533 3.297	-0.617 -0.612 -0.492
maximum deviation of 7% from the	202	26.238 26.238 26.564	53.775 56.557	44.191 45.088 46.098	250 273 273	4.808 4.808 8.808	3.081 2.865 2.649	-0.402 -0.333 -0.277
1 study, as well as lack of agreement by 3 to 10%. The entropy at 298.15 K	000 000 000 000 000 000	27.281 28.053 28.966 28.473 28.238	61.462 65.724 69.535 72.916	48.261 50.457 52.608 54.681 56.656	7.921 10.687 13.542 16.412	4.809 4.808 4.813 4.736	2217 1.785 1.353 0.923	-0.193 -0.133 -0.054
T, is hexagonal close packed, an hcp	1100	28.260	78.592	58.530	22.068	4.164 ALPHA	V	
ed value of T _m is 1135 ± 10 K. The	1300 1400 1500 1500	28.511 28.879 29.353 29.934	81.060 83.356 85.513 87.558	60.306 61.992 63.596 63.126	24.905 27.774 30.684 33.648		0000	ರರರರ
	967 888 888 888 888 888 888 888 888 888 8	30.621 31.414 32.314	89.511 91.390 93.211	66.589 67.993 69.344	36.675 39.776 42.961	ರಂದರ	ರರರ	ರರರ
hod	5000	34.433	86.722	71.907	49.629	ာ်ဝံ ဇ	ာ်ဝံ (တ်ဝံ (
ing and dilatometric curves	2125.000	35.973	98.854	73.430	54.027	U. BETA <	o. :> Liouid	1
calorimetry	2200	36.977 38.409	100.119	74.318 75.476	56.763 60.531	-21.323	0.746	
ing curve	7400 7200 7300	39.947 41.591	103.461 105.125	76.608 77.715	64.448 68.524	-22.005	3.822	-0.061 -0.080
Iron microscope	2600	43.342	106.790	78.801	72.770	-22.052	4.859	-0.098
batic calorimetry calorimetry remainal calorimetry tivity tivity								
batic calorimetry tivity tivity								
imation for β-Zr(cr) is calculated as								
								· ()

 $S^{(298.15 \text{ K})} = [47.605] \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ $T_{\text{tas}} = 2125 \pm 15 \text{ K}$

Enthalpyof Formation

The enthalpy of formation is calculated from that of the B-crystal by addition of AnH and the difference in enthalpy, H'(2125 K)-

There are no heat capacity or enthalpy studies covering the liquid region of zirconium. A constant value of C₂ = 41.84 J·K⁻¹-mol⁻¹ is assumed for the region 2125–5500 K. A glass transition is assumed at 1580 K below which extrapolated B–Zt heat capacity values are used. 4°(298.15 K), between the β-crystal and the liquid. Heat Capacity and Entropy

usion Data

The entropy is calculated in a manner similar to that used for the entralpy of formation.

The available fusion temperature and enthalpy of fusion data are summarized in the table below. We adopt $T_{los} = 2125 \pm 15 \,\mathrm{K}$ and $\Delta_{los} H^o = 20.92 \pm 6.3 \,\mathrm{kJ \cdot mol^{-1}}$.

Source	$T_{ha}Jk$	Δ _{fw} H°, kcal·mol ⁻¹
deBoer and Fast	2130	
Adenstedt 2	2113	
Oriani and Jones 3	2125 ± 2	
Deardorff and Hayes	2128	
Scott 5	2118	
Klein and Danielson 6	2118	
Rudy et al 7	2150 ± 20	
Sara *	2133 ± 15	
Rudy and Windisch?	2149 ± 4	
Elyutin et al 10		5.0 ± 0.3
Ackerman and Rauk 11	2134	
Martynyuk and Tsapkov 12		5.139

/aporization Data

The vaporization studies are summarized on the Zr(g) table. The boiling point is calculated as that temperature for which $\Delta_i G^* = 0$ for Zr(i) = Zr(g). $\Delta_{np}H^*$ is the corresponding enthalpy change. T_{np} is the temperature at which the fugacity is one bar.

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CURRENT: June 1979 Standard State Pressure = p = 0.1 MPa -2593 -2574 -2141 -1364 -1364 -1369 -080 -080 -0534 -0534 -0534 -0531 -0531 -0531 -0531 -0.150 -0.118 -0.087 -0.032 -0.032 -0.126 -0.251 -0.370 log Kr 0000 00000 00000 00000 00000 11.617 23.542 35.459 47.371 59.276 71.175 83.069 94.958 14.783 14.346 13.301 13.036 13.036 12.162 12.162 12.162 12.162 12.163 12 4.602 3.837 3.010 2.131 1.207 -560936 -560258 -560257 -559.941 -559.640 -559.075 -559.075 17.404 17 16.307 17.390 18.388 19.291 20.089 20.769 L-mol- $\Delta_i H$ ರವರದ ಪರವರದ ಪರಪಠದ ಪರವರದ ಪರ $H^{\bullet}-H^{\bullet}(T_t)$ 7.922 10.689 13.538 16.486 19.542 22.713 26.004 29.413 32.938 39.551 40.387 40.387 51.123 51.123 50.130 60.431 60 170.201 174.275 178.459 182.643 186.827 191.011 195.195 203.563 144.987 149.171 153.355 157.539 161.723 165.907 Enthalpy Reference Temperature = T, = 298.15 K S* -[G*-H*(T,)]/T 47.603 47.603 47.504 47.504 47.504 47.504 47.601 47.601 47.601 79.010 79.356 80.382 81.717 81.717 82.2016 82.214 86.514 86.514 86.713 90.139 91.226 93.236 9 100.834 101.688 102.526 103.347 104.153 104.945 105.742 106.485 107.235 107.971 51.678 55.120 58.192 60.974 65.878 70.141 73.945 80.635 83.656 86.519 89.247 91.859 96.300 96.300 96.300 96.300 96.300 101.734 104.016 106.163 108.204 110.150 113.791 115.499 117.140 118.719 120.241 121.709 124.49 125.828 125.828 128.364 129.577 130.756 131.90 131.90 135.194 135.197 137.205 138.190 138.190 138.190 138.190 141.011 141.911 141.935 27.281 28.053 30.003 31.128 31 41840 December 41.840 41.840 41.840 41.840 41.840 41.840 41.840 41.840 41.840 41.840 ť PREVIOUS. ΤÄ $\Delta_t H^o$ (298.15 K) = [17.404] kJ·mol⁻¹ $\Delta_{tus} H^o = 20.92 \pm 6.3 \text{ kJ·mol}^{-1}$

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0 to 1135 K crystal, alpha 1135 to 2125 K crystal, beta bove 2125 K liquid	Refer to the individual tables for details.
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	to 1135 K to 2125 K 2125 K

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41.840 142.792 102.859 191.679 -560.396 41.840 145.502 103.633 195.863 -560.388 24.1840 145.502 104.491 200.047 -560.287 24.1840 145.302 105.283 204.231 -559.541 4 24.1840 145.312 105.283 204.231 -559.540 5 24.1840 146.318 105.823 212.599 -559.540 24.1840 146.318 105.823 212.599 -559.375 8 24.1840 148.488 108.312 220.967 -558.809 9	4702.633	41.840	141.935	102.019	187.605	- 1		
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41.840 146,318 106,825 212,599 -559,530 75 41,840 147,720 107,575 216,783 -559,375 8 41,840 148,488 108,312 220,967 -558,809 99	2100	41.840	145.329	105.283	204.231	-559.941	47.371	-0.485
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	\$ \$ \$00 \$00 \$00	41.840	148.488	107.575 108.312	216.783 220.967	-559.075	83.069 94.958	-0.804
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251.293 252.238 253.165 254.077 254.974 255.856 256.724 256.724 256.724 256.724 257.578

114.660 118.262 121.893 125.552 129.239

231.161 231.785 232.399 233.004 233.600

37.258 37.488 37.717 37.934 38.137

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263.964 264.710

97.111 100.538 104.036 107.547 111.088

-99.431 -98.773 -98.773 -98.773 -98.773 -98.773 -98.773 -98.773 -17.094 -17.09

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8280 10953 13570 166147 18.709 22.2865 22.489 29.155 34.629 34.629 43.180 46.111

216.312 218.565 220.665 222.641 224.513

603.172 602.878 602.544 602.156 601.699

204.651 205.974 207.243 208.463 209.637

226.294 227.996 229.626 231.189

235.534 235.836 236.880 238.181 239.441

Standard State Pressure = $p^* = 0.1 \text{ MPa}$

 $H^{\bullet}-H^{\bullet}(T_{r})$

S -[G-H'(T,)]II

·K-'mol-1

203.189 188.944 183.708 181.776 181.343

164.561 171.205 176.740 181.343

21,000 22,249 24,029 25,576 26,641

-311.175 -304.976 -151.876 -120.015

567.285 560.155 553.012 545.859 538.697

608.709 609.904 609.904 609.904 610.027 610.027 610.138 610.23

181.507 185.675 189.350 192.614 192.614 192.614 204.636 208.130 211.167

25,674 27,344 27,344 27,589 27,589 22,5934 22,5934 22,510 22,754 26,048

IDEAL GAS

Enthalpy Reference Temperature = T, = 29&15 K ¥ $\Delta_t H^{\circ}(0 \text{ K}) = 608.7 \pm 8.4 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = 610.0 \pm 8.4 \text{ kJ} \cdot \text{mol}^{-1}$ S*(298.15 K) = 181.343 ± 0.04 J·K⁻¹·mol⁻¹

m Weights	2 2	6 1	1	ŀĸ
Electronic Levels and Quantum Weights State 6., cm ⁻¹ 81	0.00 570.41	1240.84	ı	51899.40 55145
Electronic State	ក្តែក្	ř <u>.</u> '	,	- 18° A

Enthalpy of Formatiom

Vapor pressures over Zr(β) and Zr(I) were measured, using the Langmuir free-vaporization method, by Zwikter,¹ Skinner et al.,² Fridorov and Smirnov³.⁴ and Koch and Anable.⁵ Trulson and Goldstein⁵ used a mass spectrometric method with a high temperature Knudson effusion source to obtain the vapor pressure for Zr(β) and Zr(l). Similarly, Ackermann and Rauh³ determined the vapor pressure for Zr(l) by a combination of mass effusion and mass spectrometric techniques. In this latter study the reported values (equation only) were obtained from wapor pressure measurements over Zr(l) saturated with tungsten. These values were then corrected for the dissolved tungsten by the corresponding mole fraction.

A plot of log p vs. I/T for the above mentioned studies reveals considerable discrepancy. The results of Fredorov and Smimov^{3 4} are an order of magnitude higher than those of Zwikker,¹ however, both studies appear inconsistent with the other studies involving Zr(β).^{2 6,7} The sublimation studies of Golubisov et al. 3 and Sumin and Peizularz¹⁰ reported $\Delta_t H^0(0 \, K)$ values of 143.1 ± 0.22 and 145.6 ± 0.4 kral·mol⁻¹ respectively. The experimental data is not given in either study.

A second and third law evaluation of seven studies yields an adopted enthalpy of formation value, $\Delta_t H^{\gamma}(298.15 \text{ K, Zr, g}) = 145.8 \pm 2.0$ kcal·mol⁻¹. This adopted value is a weighted average of four vapor pressure studies. ^{2.5 k.7} Hultgren, ⁴ using different thermodynamic functions and data available through 1967, recommended a enthalpy of foramtion (at 298.15 K) of 145.5 ± 1.0 kcal-mol⁻¹, based primarily on the data of Skinner et al.

				$\Delta_{r}H^{\circ}(298.15$	1,H°(298.15 K), kcal·mol-1	Drift	٦,
Investigator	Reaction	Τ/K	Points	2nd law	3rd law	cal·K ⁻¹ ·mol ⁻¹	kcal-mol-1
Zwikker	62	1600-2100	Ega	62.9	139.6	41.5	140.8
Skinner et al.2	æ	1949-2054	12	144.2 ± 3.0	146.5 ± 0.3	1.2 ± 1.0	147.7
Trulson and Goldstein6	ĸ	1968-2112	14	143.0 ± 3.6	142.8 ± 0.5	-0.1 ± 1.8	144.0
Federov et al. 3.	æ	1498-1723	9	59.9 ± 0.1	122.4 ± 6.8	39.0 ± 0.1	123.6
Ackermann and Rauh ⁷	æ	1975-2100	Edn	148.5	144.4	-2.0	145.6
Trulson and Goldstein ⁶	٩	2148-2274	'∞	129.7 ± 4.9	137.7 ± 0.6	3.6 ± 2.2	142.7
Koch and Anable ⁵	þ	2229-2795	91	144.5 ± 4.2	144.1 ± 2.4	-0.2 ± 1.7	149.1
Ackermann and Rauh7	ф.	2150-2500	Edn	139.6	139.3	-0.1	144.3
Reactions:	a. Zr(B	. Zr(B) = Zr(g)	b. Zr(l) = Zr(g)	Zr(g)			

Heat Capacity and Entropy

The electronic energy levels are given in the compilation by Moore. 11.12 Although we have only listed the ground state, first two excited cm-1) and the cut-off procedure up to 4000 K. The Gibbs energy function is essentially unaffected (<0.001 kcal-mol-1) up to 6000 K. The states, the highest observed excited state, and the ionization limit for Z(g), all levels listed by Moore, 11. 12 as well as estimated missing levels for n = 5 and 6, are used in our calculations. The observed levels are too numerous to list completely. Our calculations indicate that for Zr(g) the thermochemical functions are independent of the estimated missing levels for n = 5 and 6 (levels estimated and included above 52000) reported uncertainty in S°(298.15 K) is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the more exact estimation of excited states for n = 5 and 6, the consideration of states for n > 6, and the utilization of proper fill and cut-off procedures.

Continued on page 1951

PREVIOUS: June 1979 (1 Zwikker, Versl. Kon. Ak. van Wetenschappen, Amsterdam 35, 336 (1926); Proc. Roy. Ac. Amsterdam 29, 792 (1926); Physica 8, 240 (1928); and J. H. deBoer and J. D. Fack, Z. anorg. allgem. Chem. 187, 193 (1930).

Zirconium (Zr)

aff (III)

CURRENT: June 1979 (1 bar)

88 88888

 $P(Zt, g) = 55145 \pm 500 \text{ cm}^{-1}$ Zirconium (Zr)

CURRENT: March 1984 (1 bar)

	$\Delta \mu H'(0 \text{ K}) = 1268.4 \pm 25.1 \text{ kJ·mol}^{-}$	Δ _t H*(298.15 K) = [1276.563] kJ·mol ⁻
19/7r ⁺ a) = 105000 + 100 cm ⁻¹	# (4, 6) - 10,500 - 100 cill	$S'(29815 \text{ K}) = 183.639 \pm 0.04 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$

IDEAL GAS

Zirconium, Ion (Zr")

)°HΔ)°HΔ	iantum Weights	4	9 1	∞ **	01 1	ı	1	ı	12
	Electronic Levels and Quantum Weights State e., cm ⁻¹ 8,	00.0	314.67	763.44	1322.91	1	1		91737.40
'-mol-'	Electro State	F ₃₂	Î,	Fra	Fyz	1	ı	1	² H ₁ IV12

Enthalpy of Formation

 $\Delta H^{*}(Z^{2}, g, 0 \text{ K})$ is calculated from $\Delta H^{*}(Z_{*}, g, 0 \text{ K})^{1}$ using the spectroscopic value of IP(Z_{*}) = 55145 ± 5 cm⁻¹ (659.68 ± 0.06 kJ·mol⁻¹) from Moore. The ionization limit is converted from cm⁻¹ to kJ·mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ cm⁻¹, which is derived from the 1973 CODATA fundamental constants.3 Rosenstock et al. and Levin and Lias have summarized additional ionization and appearanc potential data.

 $\Delta H^{*}(ZT^{*}, g. 298.15 \text{ K})$ is calculated from $\Delta H^{*}(Zt, g. 0 \text{ K})$ by using IP(Zt) with JANAF¹ enthalpies, $H^{*}(0 \text{ K}) + H^{*}(298.15 \text{ K})$, for Zt(g), and e⁻(g). $\Delta H^{*}(Zt \to Zt^{*} + e^{-}, 298.15 \text{ K})$ differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock et al. $^{4}\Delta H^{*}(298.15 \text{ K})$ should be changed by $^{-}6.197 \text{ k} \cdot \text{H} \cdot \text{mol}^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

states, the highest observed excited state, and the ionization limit for Zr'(g), all levels listed by Moore, 28 as well as estimated missing level for n = 5 and 6, are used in our calculations. The observed levels are too numerous to list completely. Our calculations indicate that for Z'/g the thermochemical functions are independent of the estimated missing levels for n = 5 and 6 (levels estimated and included above 90000 cm-1) and the cut-off procedure up to 6000 K. The Gibbs energy function is essentially unaffected (<0.001 cal-mol-1.K-1) up to 12000 K. The reported uncertainty in S°(298.15 K) is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the more exact estimation of excited states for n = 5 and 6, the consideration of states The electronic energy levels are given in the compilations by Moore. 26 Although we have only listed the ground state, first three excites for n>6, and the utilization of proper fill and cut-off procedures.7

References

JANAF Thermochemical Tables: Zr(g), 6-30-79; e⁻(g), 3-31-82.
 E. Moore, U.S. Nat. Bur. Stand, NSRDS-NBS-34, 8 pp. (1970).
 E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
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-1 1-1 1 30 + 1 8501 - VA Wa	C-chalan D			1 2				
(98.15 K) = [1276.563] kJ·mol ⁻¹		CICI CINC 1	J·K-'mol'	J.K. imol.		Mandard Stat	Standard State Pressure = p = 0.1 MPa	7 = 0.1 MPs
	τÆ	ະ	S -[G	-[G*-H*(T,)]/T	$H^{\bullet}-H^{\bullet}(T_{\bullet})$	Δ,Η*	₽ _G	log K,
	-8888	23.495 26.127 26.127	154.699 164.776 164.776	INFINITE 208.027 192.014 186.207	-7.472 -5.333 -4.086 -2.743	1268.391		
	28.15	28.282	183.639	183.639	00°	1276.563	1227.145	-214.991
	33	28.288	183.814	183,640	.052	1276.607	1226.838	-213.612
	2 3	28.280	191.965	184.751	2.886 4.296	1278.959	1209.892	-157.996 -139.430
	8 8	27.905	198.238	186.846	5.696	1281.224	1192.361	-124.565
	<u></u>	27.268	207.510	191.505	11204	1285.431	1156.054	-86266
	888	27.232	214.348	195.853	16.646	1289.233	1118.583	-64.921
1-10m-11000 + 000571-m-1-1	1200	27.502	219.837	199.731	22.117	1292.634	1080,300	-51.299
5 kJ cm ⁻¹ , which is derived from tional ionization and amearance	1300 1400 1500 1500	27.803 27.928 28.031	224.456 226.522 228.452	203.189	30.435	1292.452	1041.959	-41.866 -38.154 -14.932
11 K) H°(708 IS K) for Zr(a)	1600 1700	28.110	230.264	207.739	36.040	1298.179	983.530	-32.109
inclusion of these enthalpies and	081	28.208	233.581	210.429 211.688	41.673	1301.683	943.985 924.069	-27.394
I if it is to be used in the ion	2000	28.244	236.555	212.896	47.319	1304.818	904.069	-23.612
	2300	28.28 28.28 22.28 22.28	239.247 239.247 240.502	214.055 215.171 216.245	50.144 52.968 55.791	1306.218 1286.168 1286.886	883.997 864.606 845.428	-21.988 -20.528 -19.200
ground state, first three excited	2400 2500	28.208 28.187	241.703 242.854	217.281 218.281	58.613 61.433	1287.602 1288.316	826.219 806.980	-17.982 -16.861
well as estimated missing levels	2600 2700	28.164 28.139	243.959 245.022	219.248 220.183	64.250 67.066	1289.028	787.713	-15.825
rated and included above 90000	7800 2800 2800 2800 2800	28.087	246.045	221.088 221.966	69.878	1290.445	749.097	-13.975 -13.144
tal constants Extension of these	3100	28.033	248.902	771644	28.4%	202.162.1	710.380	-12.369
and 6, the consideration of states	3300	28,006	249.792	224.447	81.102	1293.248	671.569	-10.962
	3400 3500	27.951 27.924	251.488 252.298	225.989 226.729	86.698 89.492	1294.633	632,672	-9.720 -9.151
	3600	27.897	253.084	227.450	92.283	1296.007	593.693	-8.614
	3808	27.842	254.591	228.839	728.79	1297.370	554.639	-7.624
	88	27.789	256.018	230.163	103.420	1298.722	515.513	-6.732
	450 60 60 60 60 60 60 60 60 60 60 60 60 60	27.763 27.737	256.70 4 257.372	230.802 231.426	106.197	1299.395	495.924	-6.318
tume II, 1952]. 8, (1978).	84 88 88 88	27.712 27.687 27.664	288.02 258.661 259.283	232.038 232.635 233.221	111.745	1300.731 1301.396 1302.058	456.698 437.062 417.410	-5.548 -5.189 -4.845
	4600 4700	27.641 27.619	259.891 260.485	233.794	120.048	1302.718	397.744	-4517
	888 888 888	27.599 27.579 27.561	261.067 261.636 262.193	234.906 235.446 735.975	125.571 128.330 131.087	743.094 744.096 745.070	362.203	-4.026 -3.861
	2100	27.545	262.738	236.494	133.843	746.044	346.576	-3.550
	2300	27.530 27.517	263.273 263.797	237,004	136.596	746.994	338.734	-3.403
	2500	27.495	264.311 264.816	23.480	142.100	748.852 749.763	322.997	-3.124
	200 200 200 200 200 200 200 200 200 200	27.488 27.481	265.311 265.798	238.954 239.421	147.599	750.664	307.191	-2.865
	2800	27.475	266.745	240,331	155.843	753.322	283.363	-2.624
								•

PREVIOUS: June 1979 (1 atm)