Литературные данные к вычислительному практикуму по физической химии

РАСЧЕТ ТЕРМОДИНАМИЧЕСКИХ ФУНКЦИЙ ПО РЕЗУЛЬТАТАМ ИЗМЕРЕНИЙ ТЕПЛОЕМКОСТИ

Москва, 2012

Литературные данные для $Na_2Er(MoO_4)(PO_4)$

Table 3. Smoothed thermodynamic functions for $Na_2Er(MoO_4)(PO_4)$

T, K	$C_p^0(T)$	$S^0(T)$	$H^0(T)-H^0(0)$, J/mol	$\Phi^0(T)$, J/(K mol)	T, K	$C_p^0(T)$	$S^0(T)$	$H^0(T)-H^0(0)$, J/mol	$\Phi^0(T)$, J/(K mol)
	J/(K mol)					J/(K mol			
8	3.277	1.238	7.633	0.2842	140	163.7	158.7	12250	71.21
10	5.080	2.159	15.96	0.5621	150	170.9	170.2	13920	77.43
12	7.078	3.258	28.10	0.9164	160	177.8	181.5	15660	83.58
14	9.259	4.510	44.41	1.338	170	184.3	192.4	17470	89.66
16	11.61	5.898	65.26	1.819	180	190.6	203.2	19350	95.67
18	14.12	7.408	90.97	2.355	190	196.4	213.6	21280	101.6
20	16.76	9.031	121.8	2.940	200	202.0	223.8	23280	107.5
25	23.91	13.53	223.3	4.597	210	207.1	233.8	25320	113.2
30	31.65	18.56	362.0	6.498	220	212.0	243.6	27420	118.9
35	39.76	24.05	540.4	8.608	230	216.6	253.1	29560	124.6
40	48.07	29.90	759.9	10.90	240	221.0	262.4	31750	130.1
45	56.42	36.04	1021	13.35	250	225.2	271.5	33980	135.6
50	64.67	42.41	1324	15.94	260	229.3	280.4	36250	141.0
60	80.51	55.62	2051	21.44	270	233.3	289.2	38570	146.3
70	95.07	69.14	2930	27.29	280	237.1	297.7	40920	151.6
80	108.1	82.71	3947	33.37	290	240.6	306.1	43310	156.8
90	119.8	96.13	5088	39.60	300	243.9	314.3	45730	161.9
100	130.1	109.3	6338	45.92	310	246.9	322.4	48180	166.9
110	139.5	122.1	7687	52.27	320	249.6	330.2	50670	171.9
120	148.1	134.7	9126	58.61	330	252.4	338.0	53180	176.8
130	156.1	146.8	10650	64.93	340	255.9	345.5	55720	181.7

Low-Temperature Heat Capacity of Sodium Erbium Molybdophosphate $Na_2Er(MoO_4)(PO_4)$

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Литературные данные для Ga_2Se_3

Heat Capacity and Thermodynamic Functi of Ga_2Se_3 from 14 to 320 K

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Table 2. Smoothed thermodynamic data for Ga_2Se_3

T, K	$C_p^0(T)$	$S^0(T)$	$\Phi^0(T)$	$H^0(T) - H^0(0)$, J/mol
	J/(K mol)			
15	3.477	1.209	0.304	13.56
20	9.289	3.007	0.731	45.51
25	15.02	5.697	1.444	106.3
30	20.64	8.934	2.417	195.5
35	26.14	12.53	3.601	312.5
40	31.51	16.37	4.955	456.7
45	36.71	20.39	6.446	627.3
50	41.74	24.52	8.045	823.5
60	51.19	32.97	11.49	1289
70	59.40	41.52	15.17	1844
80	67.46	50.01	19.00	2481
90	74.35	58.36	22.91	3191
100	80.45	66.52	26.86	3966
110	85.81	74.44	30.83	4797
120	90.46	82.11	34.79	5679
130	94.47	89.52	38.71	6605
140	97.92	96.65	42.60	7567
150	100.9	103.5	46.43	8561
160	103.4	110.1	50.21	9583
170	105.6	116.4	53.92	10630
180	107.6	122.5	57.56	11700
190	109.3	128.4	61.14	12780
200	110.9	134.0	64.64	13880
210	112.3	139.5	68.08	15000
220	113.7	144.7	71.44	16130
230	114.9	149.8	74.74	17270
240	116.0	154.7	77.97	18420
250	117.0	159.5	81.14	19590
260	117.9	164.1	84.24	20760
270	118.8	168.6	87.28	21950
280	119.5	172.9	90.26	23140
290	120.2	177.1	93.19	24340
298.15	120.8	180.4	95.52	25320
300	120.9	181.2	96.05	25540
310	121.5	185.2	98.86	26760
320	122.1	189.0	101.6	27970

Литературные данные для URh_3

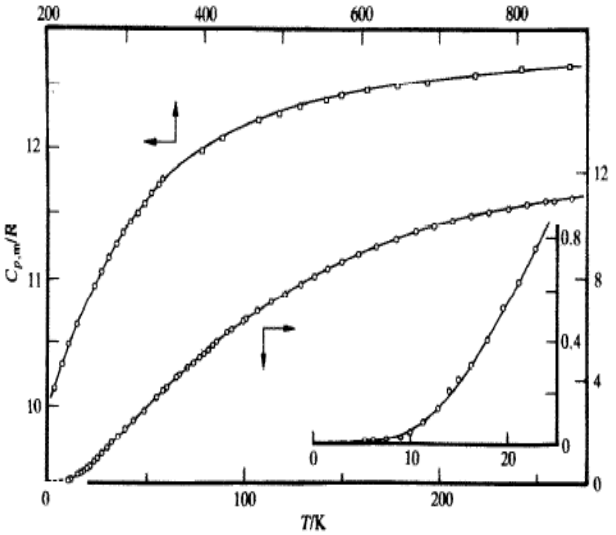

FIGURE 2. The heat capacity of URu_3. ○, Heat capacities determined in the cryogenic adiabatic calorimeter; □, heat capacities derived from enthalpy determinations.

Thermodynamics of uranium intermetallic compounds

I. Heat capacities of URu_3 and URh_3 from 5 to 850 K [a]

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J. Chem. Thermodynamics **1985**, 17, 1035–1044

TABLE 3. Thermodynamic properties of URu_3 and URh_3 ($R = 8.3143\ J \cdot K^{-1} \cdot mol^{-1}$)

$\frac{T}{K}$	$\frac{C_{p,m}}{R}$	$\frac{S^\circ_m(T)-S^\circ_m(0)}{R}$	$\frac{H^\circ_m(T)-H^\circ_m(0)}{R\,K}$	$\frac{-\{G^\circ_m(T)-H^\circ_m(0)\}}{RT}$
		URu_3		
5	0.015	0.013	0.033	0.006
10	0.053	0.032	0.186	0.014
15	0.152	0.070	0.663	0.026
20	0.356	0.138	1.879	0.044
25	0.692	0.251	4.443	0.074
30	1.147	0.416	9.001	0.116
40	2.278	0.895	25.897	0.247
50	3.610	1.548	55.406	0.439
60	4.847	2.317	97.786	0.687
70	5.951	3.149	151.90	0.979
80	6.903	4.007	216.30	1.304
90	7.703	4.868	289.45	1.652
100	8.368	5.715	369.91	2.016
120	9.372	7.335	547.92	2.769
140	10.077	8.836	742.80	3.530
160	10.602	10.217	949.82	4.281
180	11.010	11.490	1166.1	5.012
200	11.330	12.667	1389.6	5.719
220	11.578	13.760	1618.8	6.401
240	11.772	14.776	1852.4	7.057
260	11.930	15.72	2089.4	7.688
280	12.073	16.61	2329.5	8.294
300	12.210	17.45	2572.3	8.877
320	12.337	18.24	2817.8	9.438
340	12.445	18.99	3065.7	9.978
273.15	12.025	16.32	2247.0	8.089
298.15	12.198	17.38	2549.8	8.824
400	12.69	21.04	3819.7	11.49
500	13.03	23.91	5106.0	13.70
600	13.34	26.31	6424.8	15.60
700	13.62	28.39	7773.0	17.28
800	13.90	30.22	9149.3	18.79
900	14.18	31.88	10553.4	20.15

Литературные данные для IrO_2

TABLE 2. Thermodynamic properties of IrO_2 ($R = 8.3144\ J \cdot K^{-1} \cdot mol^{-1}$)

T/K	$C_{p,m}/R$	$\Delta_0^T S_m^\circ/R$	$\Delta_0^T H_m^\circ/R \cdot K$	$\Phi_m(T,0)/R$	T/K	$C_{p,m}/R$	$\Delta_0^T S_m^\circ/R$	$\Delta_0^T H_m^\circ/R \cdot K$	$\Phi_m(T,0)/R$
5	0.005	0.004	0.010	0.0018	140	3.516	2.30	207.0	0.8266
10	0.016	0.010	0.058	0.0041	160	4.034	2.809	282.6	1.0429
15	0.039	0.021	0.197	0.0077	180	4.506	3.312	368.1	1.2672
20	0.076	0.039	0.479	0.0126	200	4.941	3.810	462.6	1.4966
25	0.133	0.061	0.992	0.0195	220	5.354	4.300	565.6	1.729
30	0.212	0.090	1.843	0.0285	240	5.746	4.785	676.6	1.964
40	0.435	0.179	5.005	0.0538	260	6.105	5.257	795.2	2.199
50	0.725	0.307	10.758	0.0914	280	6.423	5.721	920.5	2.434
60	1.052	0.467	19.62	0.1403	300	6.713	6.175	1051.9	2.668
70	1.392	0.655	31.84	0.2001	320	6.992	6.210	1188.8	2.901
80	1.738	0.864	47.50	0.2698	350	7.278	7.256	1403.2	3.247
90	2.067	1.087	66.54	0.3481					
100	2.378	1.321	88.77	0.4336	273.15	6.318	5.564	876.9	2.353
120	2.961	1.80	142.22	0.6218	298.15	6.687	6.133	1039.5	2.647

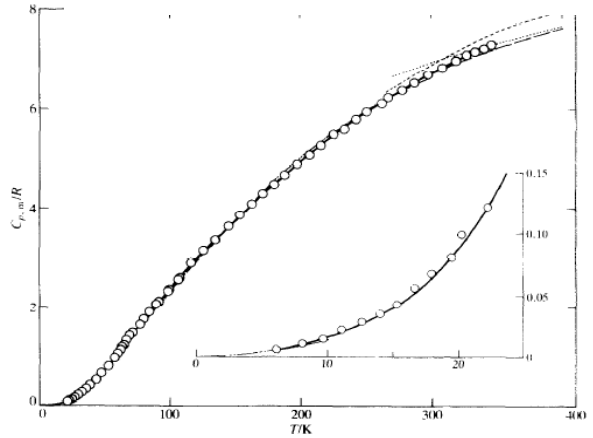

FIGURE 1. The molar heat capacity of IrO_2 over the range 0 to 400 K: —○—, this research; ····, Passenheim and McCollum;[1] - - - -, Wöhler and Jochum;[2] — — —, Cordfunke;[3] - · - ·, the estimates of Bell *et al.*[7] The molar heat capacity of isostructural TiO_2 (rutile) of Shomate[8] (50 to 300 K) is also shown: ~ · · · ~

Low-temperature heat capacity and thermodynamic functions of IrO_2[a]

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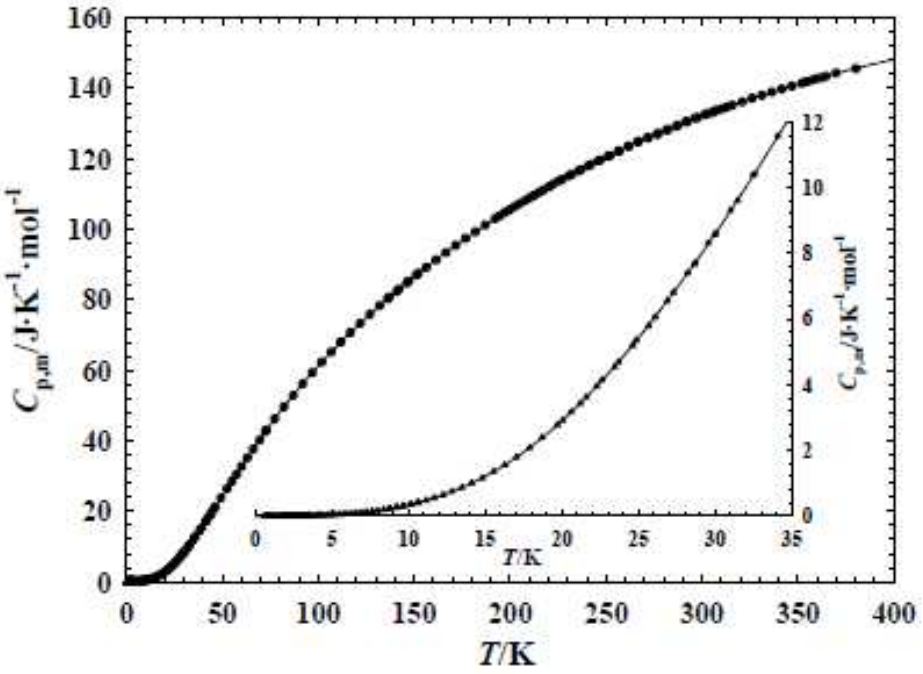
J. Chem. Thermodynamics **1987,** 19, 1227–1231

Литературные данные для Zn_2GeO_4

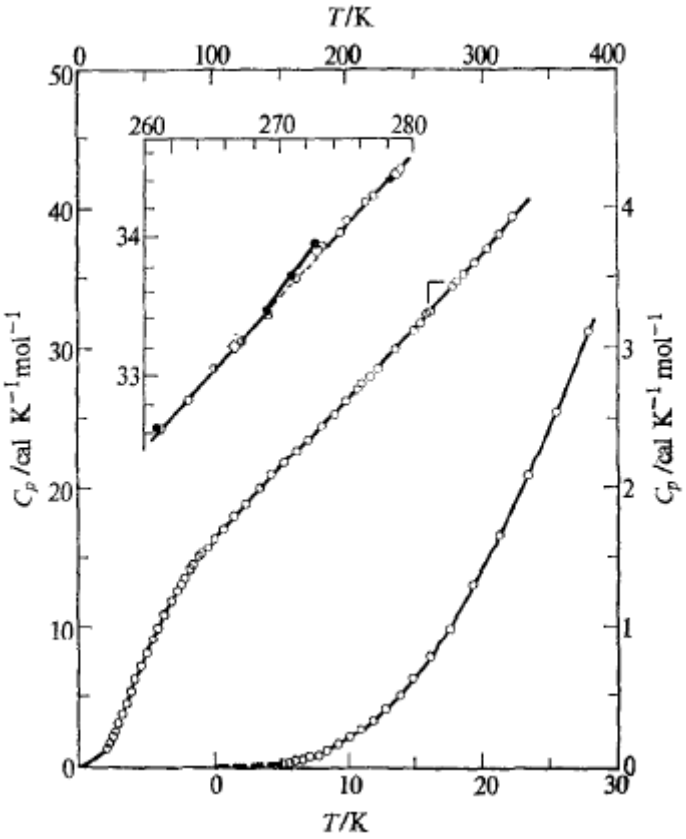


Standard molar thermodynamic functions of Zn_2GeO_4(cr)

T/K	$C^\circ_{p,m}/R$	$\Delta_0^T S^\circ_m/R$	$\Delta_0^T H^\circ_m/RT$	Φ°_m/R
5	0.004699	0.001585	0.0011654	0.0004200
10	0.041408	0.013292	0.010031	0.003261
15	0.14567	0.046906	0.035472	0.011434
20	0.34882	0.11410	0.086209	0.027894
25	0.65239	0.22284	0.16756	0.055286
30	1.0332	0.37448	0.27921	0.095270
35	1.4723	0.56615	0.41776	0.14839
40	1.9428	0.79318	0.57872	0.21446
45	2.4342	1.0502	0.75743	0.29279
50	2.9367	1.3326	0.95018	0.38246
60	3.9409	1.9571	1.3652	0.59190
70	4.9036	2.6377	1.8026	0.83503
80	5.7988	3.3517	2.2470	1.1047
90	6.6205	4.0829	2.6879	1.3949
100	7.3734	4.8199	3.1194	1.7006
110	8.0669	5.5557	3.5381	2.0176
120	8.7106	6.2855	3.9426	2.3429
130	9.3127	7.0067	4.3328	2.6740
140	9.8795	7.7178	4.7089	3.0089
150	10.415	8.4179	5.0716	3.3462
160	10.923	9.1064	5.4216	3.6848
170	11.406	9.7833	5.7596	4.0237
180	11.864	10.448	6.0861	4.3622
190	12.299	11.101	6.4017	4.6998
200	12.712	11.743	6.7070	5.0359
210	13.105	12.373	7.0024	5.3704
220	13.478	12.991	7.2883	5.7027
230	13.833	13.598	7.5652	6.0329
240	14.173	14.194	7.8335	6.3605
250	14.498	14.779	8.0937	6.6856
260	14.809	15.354	8.3460	7.0080
270	15.105	15.918	8.5909	7.3276
273.15	15.196	16.094	8.6665	7.4277
280	15.387	16.473	8.8286	7.6443
290	15.653	17.018	9.0594	7.9582
298.15	15.859	17.454	9.2425	8.2118
300	15.904	17.553	9.2834	8.2691

Heat capacities, third-law entropies and thermodynamic functions
of the negative thermal expansion material Zn2GeO4 from T = (0 to 400) K
Rebecca Stevens, Brian F. Woodfield, Juliana Boerio-Goates,
Michael K. Crawford
J. Chem. Thermodynamics 36 (2004) 349–357

Литературные данные для янтарной кислоты



Succinic acid. Heat capacities and thermodynamic properties from 5 to 328 K. An efficient drying procedure. CECIL E. VANDERZEE // J. Chem. Thwmodynamics 1970, 2, 681-687

TABLE 4. Thermodynamic functions of succinic acid

T / K	C_p / cal K^{-1} mol^{-1}	S° / cal K^{-1} mol^{-1}	$H^\circ - H_0^\circ$ / cal mol^{-1}	$-(G^\circ - H_0^\circ)/T$ / cal K^{-1} mol^{-1}
5	0.024	0.008	0.03	0.002
10	0.194	0.064	0.48	0.016
15	0.649	0.218	2.46	0.054
20	1.419	0.503	7.50	0.128
25	2.444	0.926	17.07	0.243
30	3.616	1.474	32.18	0.401
35	4.864	2.124	53.36	0.600
40	6.090	2.855	80.78	0.835
45	7.289	3.642	114.26	1.103
50	8.424	4.469	153.57	1.398
60	10.489	6.192	248.4	2.052
70	12.277	7.946	362.4	2.769
80	13.821	9.689	493.1	3.525
90	15.175	11.397	638.2	4.306
100	16.391	13.060	796.1	5.098
110	17.51	14.675	965.7	5.896
120	18.57	16.245	1146.2	6.693
130	19.60	17.772	1337.1	7.487
140	20.60	19.261	1538.1	8.275
150	21.58	20.716	1748.9	9.056
160	22.55	22.139	1970	9.839
170	23.51	23.535	2200	10.595
180	24.48	24.907	2440	11.352
190	25.44	26.256	2689	12.101
200	26.41	27.585	2949	12.842
210	27.40	28.898	3218	13.575
220	28.40	30.195	3497	14.301
230	29.41	31.480	3786	15.020
240	30.44	32.753	4085	15.733
250	31.47	34.017	4395	16.439
260	32.51	35.27	4714	17.14
270	33.56	36.52	5045	17.83
280	34.61	37.76	5386	18.52
290	35.67	38.99	5737	19.21
300	36.75	40.22	6099	19.89
310	37.86	41.44	6472	20.56
320	38.98	42.66	6856	21.23
273.15	33.89	36.91	5151	18.05
298.15	36.55	39.99	6031	19.76

Литературные данные для моногидрата лимонной кислоты

temp., °K	C (abs. J deg.$^{-1}$g^{-1})	$S^{\circ}_{T}-S^{\circ}_{\circ}$ (abs. J deg.$^{-1}$g^{-1})	$H^{\circ}_{T}-H^{\circ}_{\circ}$ (abs. J g^{-1})
0	0	0	0
10	0·0085	0·0034	0·0267
20	0·0594	0·0218	0·3203
30	0·1324	0·0601	1·301
40	0·2001	0·1073	2·950
50	0·2676	0·1593	5·289
60	0·3322	0·2136	8·292
70	0·3919	0·2694	11·92
80	0·4444	0·3252	16·10
90	0·4917	0·3803	20·79
100	0·5329	0·4344	25·92
110	0·5711	0·4870	31·44
120	0·6107	0·5384	37·35
130	0·6491	0·5888	43·65
140	0·6846	0·6381	50·32
150	0·7196	0·6865	57·33
160	0·7552	0·7341	64·71
170	0·7917	0·7810	72·44
180	0·8280	0·8273	80·54
190	0·8651	0·8730	89·01
200	0 9042	0·9184	97·85
210	0·9437	0·9635	107·1
220	0·9816	1·008	116·7
230	1·017	1·053	126·7
240	1·055	1·097	137·1
250	1·093	1·141	147·8
260	1·132	1·184	158·9
270	1·170	1·228	170·4
273·15	1·182	1·241	174·2
280	1·207	1·271	182·3
290	1·245	1·314	194·6
298·15	1·276	1·349	204·9
300	1·282	1·357	207·2