SUPPORTING INFORMATION (SI)

Thermodynamics and crystal structures of krautite, $Mn[AsO_3(OH)]\cdot H_2O$, koritnigite, $Zn[AsO_3(OH)]\cdot H_2O$, and cobaltkoritnigite, $Co[AsO_3(OH)]\cdot H_2O$

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Table S1. Complete bond-valence analysis for the synthetic koritnigite (all values given in valence units, *vu*).

	As1	As2	As3	As4	Zn1	Zn2	Zn3	Zn4	H1O20	H2O20	H1O17	H2O17	H1O15	H2O15	H1O11	h2o11	H1O16	H1O14	H1O18	H1O12	BV-H	BV+H
O1	1.30				0.70																2.00	2.00
O2		1.34			0.28			0.41													2.02	2.02
O3			1.26			0.31	0.37														1.94	1.94
O4	1.27				0.37			0.34													1.97	1.97
O5		1.31			0.34															0.18	1.66	1.84
O6				1.31		0.38	0.31														2.00	2.00
O7				1.35		0.68															2.03	2.03
O8		1.26						0.72													1.98	1.98
O9			1.31				0.70														2.01	2.01
O10				1.32					0.14						0.11		0.16				1.32	1.73
O11						0.36						0.07			0.83	0.83					0.36	2.08
O12	1.13							0.12												0.81	1.25	2.06
O13	1.30						0.13				0.10		0.16						0.20		1.42	1.89
O14				1.05														0.83			1.05	1.88
O15					0.35					0.09			0.83	0.83							0.35	2.09
O16		1.18												0.12			0.83				1.18	2.12
O17								0.41			0.83	0.86									0.41	2.10
O18			1.14													0.15			0.81		1.14	2.09
O19			1.22			0.34												0.21			1.55	1.76
O20							0.38		0.83	0.84											0.38	2.05
	4.99	5.09	4.93	5.03	2.03	2.07	1.89	2.00	0.97	0.94	0.93	0.93	0.98	0.95	0.94	0.97	0.99	1.03	1.01	0.99		

BV–H – bond-valence sum without contribution of the H-bonds; BV+H – sum of bond-valences with H-bonds considered.

Table S2. Selected interatomic distances (in Å) and polyhedral-distortion measures for the structure of synthetic koritnigite.

Zn1–O1^{v}	2.060(7)	Zn3–O3	2.064(7)
Zn1–O1^{iii}	2.119(9)	Zn3–O6^{vii}	2.127(8)
Zn1–O2^{vi}	2.178(9)	Zn3–O9^{v}	2.105(6)
Zn1–O4	2.064(7)	Zn3–O9^{viii}	2.073(7)
Zn1–O5	2.094(8)	Zn3–O14^{v}	2.480(7)
Zn1–O15	2.088(8)	Zn3–O20	2.055(8)
<Zn1–O>	2.100	<Zn3–O>	2.151
Octahedral distortion	3.60	Octahedral distortion	48.21
Effective coordination number	5.921	Effective coordination number	4.971
Zn2–O3^{vii}	2.133(8)	Zn4–O2	2.030(7)
Zn2–O6	2.059(6)	Zn4–O4^{vi}	2.100(9)
Zn2–O7^{v}	2.078(6)	Zn4–O8^{v}	2.098(7)
Zn2–O7^{iv}	2.113(8)	Zn4–O8^{ix}	2.056(9)
Zn2–O11	2.071(9)	Zn4–O12^{v}	2.481(9)
Zn2–O19	2.100(7)	Zn4–O17	2.021(11)
<Zn2–O>	2.092	<Zn4–O>	2.131
Octahedral distortion	1.49	Octahedral distortion	55.96
Effective coordination number	5.968	Effective coordination number	4.953
As1–O1	1.671(8)	As3–O3	1.683(7)
As1–O4	1.682(7)	As3–O9	1.669(7)
As1–O12	1.723(8)	As3–O18	1.719(9)
As1–O13	1.673(9)	As3–O19	1.696(7)
<As1–O>	1.687	<As3–O>	1.692
As2–O2	1.662(8)	As4–O6	1.670(6)
As2–O5	1.669(8)	As4–O7	1.660(7)
As2–O8	1.684(8)	As4–O10	1.668(8)
As2–O16	1.708(8)	As4–O14	1.747(7)
<As2–O>	1.681	<As4–O>	1.686

Symmetry codes: (iii) –*x*, –*y*, –*z*; (iv) –*x*+1, –*y*–1, –*z*–1; (v) *x*, *y*, *z*–1; (vi) –*x*, –*y*, –*z*–1; (vii) –*x*+1, –*y*–1, –*z*–2; (viii) –*x*+2, –*y*–1, –*z*–2; 11 (ix) –*x*+1, –*y*, –*z*–1. ECoN – effective coordination number (Hoppe 1979); distortion – octahedral distortion (Brown and Shannon 1973).

Table S3. Hydrogen-bond geometry (in Å and °) in the structure of synthetic koritnigite.

D–H···*A*	*D*–H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*–H···*A* (°)
O20–H1O20···O10^{xvi}	1.00(3)	1.75(3)	2.724(11)	163(5)
O20–H2O20···O15^{xvi}	0.99(5)	1.93(5)	2.905(11)	170(5)
O17–H1O17···O13^{xvi}	1.00(4)	1.89(4)	2.762(11)	143(6)
O17–H2O17···O11	0.98(6)	2.08(6)	2.881(14)	138(5)
O15–H1O15···O13^{v}	1.00(4)	1.71(3)	2.674(10)	162(7)
O15–H2O15···O16^{xiv}	1.01(5)	1.82(4)	2.670(11)	139(5)
O11–H1O11···O10^{v}	1.00(3)	1.86(3)	2.752(9)	147(5)
O11–H2O11···O18^{xiv}	1.00(3)	1.74(3)	2.713(11)	163(6)
O16–H1O16···O10	1.00(5)	1.69(5)	2.590(11)	148(4)
O14–H1O14···O19	0.999(17)	1.59(3)	2.543(8)	157(6)
O18–H1O18···O13^{xvi}	1.01(4)	1.60(5)	2.563(13)	158(5)
O12–H1O12···O5	1.01(4)	1.64(3)	2.554(10)	149(7)

Symmetry codes: (v) *x*, *y*, *z*–1; (xiv) *x*–1, *y*, *z*; (xvi) *x*+1, *y*, *z*–1.

Table S4. Complete bond-valence analysis for the synthetic krautite (all values given in valence units, *vu*).

	As1	As2	As3	As4	Mn1	Mn2	Mn3	Mn4	H1O20	H2O20	H1O13	H2O13	H1O10	H2O10	H1O7	H2O7	H1O18	H1O17	H1O5	BV-H	BV+H
O1			1.27		0.34			0.35												1.97	1.97
O2		1.23			0.32														0.20	1.55	1.75
O3			1.29		0.37		0.34													2.00	2.00
O4		1.27				0.37	0.35													1.99	1.99
O5			1.05			0.28													0.83	1.33	2.15
O6		1.27				0.41		0.32												2.00	2.00
O7					0.32				0.10						0.86	0.86				0.32	2.14
O8	1.17											0.13								1.17	1.30*
O9			1.34											0.13		0.15				1.34	1.62
O10						0.43							0.91	0.91						0.43	2.24
O11				1.28		0.34	0.35													1.97	1.97
O12				1.34						0.12	0.15						0.18			1.34	1.79
O13							0.34				0.86	0.86								0.34	2.07
O14				1.30	0.34		0.37													2.01	2.01
O15	1.31					0.31		0.41												2.03	2.03
O16	1.30						0.29											0.20		1.58	1.78
O17				1.05				0.28										0.83		1.32	2.15
O18		1.17											0.02		0.12		0.83			1.17	2.13
O19	1.27				0.35			0.37												1.99	1.99
O20								0.41	0.86	0.86										0.41	2.14
	5.04	4.95	4.95	4.98	2.04	2.13	2.04	2.13	0.96	0.98	1.01	1.00	0.93	1.04	0.98	1.01	1.01	1.02	1.03		

BV–H – bond-valence sum without contribution of the H-bonds; BV+H – sum of bond-valences with H-bonds considered. * - considerably underbonded O atom = it is due to somwe of the H atoms positionally incorrectly refined – O8 should receive additional weak H bond.

Table S5. Selected interatomic distances (in Å) and polyhedral-distortion measures for the structure of synthetic krautite.

Mn1–O1^{vi}	2.184(5)	Mn3–O3	2.187(5)
Mn1–O2^{i}	2.220(4)	Mn3–O4	2.182(5)
Mn1–O3	2.156(5)	Mn3–O11^{iv}	2.179(4)
Mn1–O7	2.221(5)	Mn3–O13	2.192(5)
Mn1–O14	2.188(5)	Mn3–O14	2.155(4)
Mn1–O19	2.173(5)	Mn3–O16^{ii}	2.257(4)
<Mn1–O>	2.190	<Mn3–O>	2.192
Octahedral distortion	1.16	Octahedral distortion	2.04
Effective coordination number	5.975	Effective coordination number	5.957
Mn2–O4^{vi}	2.159(4)	Mn4–O1	2.180(5)
Mn2–O5^{vii}	2.277(4)	Mn4–O6^{viii}	2.219(5)
Mn2–O6	2.109(4)	Mn4–O15	2.107(4)
Mn2–O10	2.095(6)	Mn4–O17^{viii}	2.278(4)
Mn2–O11	2.188(5)	Mn4–O19^{iv}	2.159(4)
Mn2–O15^{vii}	2.229(5)	Mn4–O20	2.116(5)
<Mn2–O>	2.176	<Mn4–O>	2.177
Octahedral distortion	8.62	Octahedral distortion	7.36
Effective coordination number	5.791	Effective coordination number	5.830
As1–O8	1.711(6)	As3–O1	1.680(5)
As1–O15	1.671(4)	As3–O3	1.676(5)
As1–O16	1.674(4)	As3–O5	1.748(4)
As1–O19	1.680(4)	As3–O9	1.663(5)
<As1–O>	1.684	<As3–O>	1.692
As2–O2	1.692(4)	As4–O11	1.677(4)
As2–O4	1.680(4)	As4–O12	1.661(5)
As2–O6	1.680(4)	As4–O14	1.672(4)
As2–O18	1.710(6)	As4–O17	1.748(4)
<As2–O>	1.691	<As4–O>	1.690

Symmetry codes: (iii) –*x*, –*y*, –*z*; (iv) –*x*+1, –*y*–1, –*z*–1; (v) *x*, *y*, *z*–1; (vi) –*x*, –*y*, –*z*–1; (vii) –*x*+1, –*y*–1, –*z*–2; (viii) –*x*+2, –*y*–1, –*z*–2; 11 (ix) –*x*+1, –*y*, –*z*–1. ECoN – effective coordination number (Hoppe 1979); distortion – octahedral distortion (Brown and Shannon 1973).

Table S6. Hydrogen-bond geometry (in Å and °) in the structure of synthetic krautite.

D–H···*A*	*D*–H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*–H···*A* (°)
O5–H1O5···O2i	0.998(18)	1.595(17)	2.589(6)	174(7)
O7–H1O7···O18	0.98(2)	1.84(3)	2.799(7)	166(7)
O7–H2O7···O9^{vi}	0.98(2)	1.729(19)	2.686(7)	164(7)
O8–H1O8···O9^{x}	1.01(6)	1.66(5)	2.556(8)	147(6)
O10–H1O10···O18	0.96(5)	2.60(6)	3.227(7)	123(4)
O10–H2O10···O9^{vi}	0.96(2)	1.794(19)	2.698(7)	157(5)
O13–H1O13···O12^{iv}	0.98(3)	1.74(3)	2.678(7)	159(7)
O13–H2oO13···O8	0.98(4)	1.78(3)	2.731(7)	165(5)
O17–H1O17···O16^{ii}	1.00(3)	1.61(2)	2.586(6)	164(7)
O18–H1O18···O12^{xi}	1.00(5)	1.64(5)	2.586(8)	155(5)
O20–H1O20···O7^{x}	0.98(2)	1.91(19)	2.888(6)	176(4)
O20–H2O20···O12^{iv}	0.98(2)	1.83(18)	2.717(5)	149(4)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*–1, *y*, *z*; (iv) *x*, *y*, *z*+1; (vi) *x*, *y*, *z*–1; (x) –*x*+2, *y*+1/2, –*z*+2; (xi) –*x*+1, *y*–1/2, –*z*+1.

Table S7. Measured values of molar heat capacity for koritnigite, $Zn[AsO_3(OH)]\cdot H_2O$.

T	C_p	T	C_p	T	C_p	T	C_p	T
K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K
2.20396	0.032472	6.82051	0.198255	22.0908	4.52815	72.0196	43.6831	235.026
2.20482	0.032485	6.82289	0.198875	22.0946	4.50673	72.0304	43.6102	235.141
2.20715	0.032597	6.82453	0.198613	22.1079	4.50192	72.0335	43.8734	235.151
2.38174	0.038023	7.39744	0.241132	24.0321	5.69179	78.3649	48.5679	255.724
2.38346	0.038068	7.39986	0.241705	24.0332	5.56257	78.3798	48.5633	255.89
2.38498	0.038008	7.40177	0.241419	24.0353	5.566	78.3852	48.8704	255.904
2.57613	0.045	8.04126	0.299064	26.132	6.81616	85.2738	54.0277	278.221
2.57716	0.045094	8.04297	0.298288	26.1498	6.80944	85.2764	53.8307	278.46
2.58006	0.045204	8.04732	0.299026	26.1703	6.72866	85.2917	54.0943	278.48
2.78818	0.054279	8.74214	0.372561	28.4504	8.28006	92.8054	58.8503	303.003
2.78966	0.054346	8.74353	0.371471	28.4521	8.27132	92.8132	58.9552	303.018
2.79242	0.054491	8.74588	0.372703	28.4546	8.29975	92.8219	59.268	303.025
3.01217	0.065129	9.51129	0.467651	30.9466	10.0013	100.979	64.6728	
3.01784	0.065223	9.51216	0.468844	30.9607	9.97472	100.994	64.6545	
3.01974	0.065356	9.51623	0.468411	30.962	9.99753	101.003	65.0694	
3.25832	0.065765	10.3395	0.591035	33.6729	12.0144	109.893	70.8435	
3.26509	0.066002	10.343	0.588595	33.6825	12.0185	109.903	70.7253	
3.267	0.066006	10.3499	0.589705	33.6828	12.0144	109.914	70.9367	
3.53513	0.067044	11.252	0.746768	36.6406	14.309	119.582	76.9091	
3.54022	0.067009	11.2525	0.744478	36.6452	14.3071	119.587	76.8271	
3.5424	0.067025	11.2583	0.746087	36.6502	14.341	119.592	76.7552	
3.83328	0.07028	12.2366	0.943454	39.8668	16.9416	130.129	83.1821	
3.83494	0.070177	12.2382	0.942888	39.8686	17.0788	130.135	83.1409	
3.83667	0.070144	12.2447	0.94197	39.8807	16.9408	130.139	83.0696	
4.15487	0.077448	13.32	1.19228	43.3777	19.8323	141.591	89.2007	
4.15501	0.077383	13.3251	1.18762	43.3812	19.9946	141.609	89.2264	
4.15786	0.077358	13.3319	1.19026	43.394	19.8295	141.613	89.6843	
4.5064	0.087155	14.4879	1.49852	47.2115	23.056	154.082	95.9775	
4.50647	0.087172	14.4921	1.49535	47.2219	23.1953	154.089	95.8149	
4.50841	0.087399	14.5018	1.49897	47.2246	23.0531	154.113	95.7983	
4.88817	0.099682	15.7679	1.88838	51.3709	26.5686	167.678	102.707	
4.88905	0.09956	15.7743	1.88527	51.3808	26.7627	167.678	103.034	
4.89154	0.099924	15.7744	1.8839	51.385	26.568	167.698	102.843	
5.30524	0.1161	17.1606	2.36577	55.8985	30.4112	182.463	109.842	
5.30623	0.115617	17.1648	2.37245	55.9085	30.626	182.469	109.927	
5.30948	0.115704	17.1722	2.3649	55.9137	30.4154	182.48	109.747	
5.75959	0.136054	18.6488	2.93451	60.823	34.5421	198.599	116.983	
5.76239	0.136342	18.6687	2.94012	60.8317	34.8372	198.605	116.895	
5.7633	0.136253	18.6735	2.94944	60.8381	34.535	198.62	116.72	
6.26348	0.163164	20.3088	3.65196	66.1857	38.9649	216.01	124.258	
6.26514	0.163984	20.3124	3.66112	66.1951	38.9498	216.094	124.108	
6.28384	0.165248	20.3325	3.63564	66.1953	39.1966	216.098	124.23	

Table S8. Molar thermodynamic functions for koritnigite, $Zn[AsO_3(OH)]\cdot H_2O$, calculated from smoothed heat capacity.

T	C_p	H_T	$(H_T-H_0)/T$	S_T	G_T	$-(G_T-G_0)/T$
K	$J\cdot K^{-1}$	J	$J\cdot K^{-1}$	$J\cdot K^{-1}$	J	$J\cdot K^{-1}$
0	0	0	NaN	0	0	NaN
5	0.1036	0.2124	0.04247	0.06574	-0.1163	0.02326
10	0.5366	1.58	0.158	0.239	-0.8098	0.08098
15	1.646	6.727	0.4485	0.6414	-2.893	0.1929
20	3.515	19.31	0.9655	1.352	-7.74	0.387
25	6.119	43.11	1.724	2.404	-16.99	0.6795
30	9.341	81.53	2.718	3.796	-32.35	1.078
35	13.03	137.3	3.923	5.508	-55.48	1.585
40	17.03	212.3	5.309	7.506	-87.9	2.198
45	21.22	307.9	6.843	9.753	-131	2.91
50	25.48	424.7	8.494	12.21	-185.8	3.716
55	29.75	562.8	10.23	14.84	-253.3	4.606
60	33.96	722.1	12.03	17.61	-334.4	5.573
65	38.09	902.2	13.88	20.49	-429.6	6.609
70	42.12	1103	15.75	23.46	-539.4	7.706
75	46.05	1323	17.64	26.5	-664.3	8.858
80	49.87	1563	19.54	29.6	-804.5	10.06
85	53.59	1822	21.43	32.73	-960.3	11.3
90	57.21	2099	23.32	35.9	-1132	12.58
95	60.74	2394	25.2	39.08	-1319	13.89
100	64.18	2706	27.06	42.29	-1523	15.23
110	70.81	3381	30.74	48.72	-1978	17.98
120	77.11	4121	34.34	55.15	-2497	20.81
130	83.01	4922	37.86	61.56	-3081	23.7
140	88.53	5780	41.29	67.92	-3728	26.63
150	93.81	6692	44.61	74.21	-4439	29.59
160	98.92	7656	47.85	80.42	-5212	32.58
170	103.9	8670	51	86.57	-6047	35.57
180	108.7	9733	54.07	92.64	-6943	38.57
190	113.2	10840	57.07	98.64	-7900	41.58
200	117.6	12000	59.98	104.6	-8916	44.58
210	121.7	13190	62.83	110.4	-9991	47.57
220	125.7	14430	65.6	116.2	-11120	50.56
230	129.6	15710	68.29	121.8	-12310	53.54
240	133.4	17020	70.93	127.4	-13560	56.5
250	137.2	18380	73.5	133	-14860	59.45
260	141.1	19770	76.03	138.4	-16220	62.38
270	144.8	21200	78.51	143.8	-17630	65.3
273.15	146	21660	79.28	145.5	-18090	66.21
280	148.4	22660	80.94	149.1	-19090	68.19
290	151.8	24170	83.33	154.4	-20610	71.08
298.15	154.4	25410	85.23	158.6	-21890	73.41
300	155	25700	85.66	159.6	-22180	73.94

Table S9. Measured values of molar heat capacity for krautite, $Mn[AsO_3(OH)]\cdot H_2O$.

T	C_p	T	C_p	T	C_p	T	C_p	T	C_p
K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$	K	$J\cdot K^{-1}$
2.39647	6.11276	7.39963	4.73841	24.022	6.75219	78.3427	50.2247	255.706	143.881
2.39661	6.11416	7.4125	4.72723	24.0304	6.74811	78.3626	50.644	255.868	143.744
2.40326	6.14759	7.4163	4.72377	24.0529	6.75958	78.3666	50.2589	255.868	143.849
2.59059	7.24859	8.04411	4.49327	26.1303	7.90294	85.2551	56.1271	278.201	152.485
2.59092	7.24935	8.0574	4.47587	26.1459	7.91781	85.2633	55.7524	278.429	152.459
2.60244	7.32727	8.06211	4.4763	26.1595	7.79592	85.2715	55.6061	278.436	152.226
2.80188	8.76145	8.74773	4.26378	28.4328	9.28532	92.7668	61.3645	302.963	159.87
2.80216	8.76372	8.75952	4.25447	28.4431	9.28505	92.7761	61.2975	302.968	160.154
2.81197	8.84032	8.76437	4.25154	28.447	9.29336	92.7854	61.0168	302.973	159.931
3.01767	10.3679	9.51258	4.07975	30.9406	10.9494	100.937	67.0605		
3.03004	10.3731	9.5257	4.06702	30.9509	10.9582	100.952	67.0347		
3.03061	10.373	9.53137	4.07125	30.9521	10.9537	100.953	67.248		
3.26451	9.2994	10.3471	3.93316	33.6696	12.936	109.849	73.2179		
3.28182	9.2738	10.3567	3.9246	33.6793	12.9357	109.856	73.2433		
3.28269	9.27135	10.3646	3.92484	33.6802	12.9847	109.87	73.2297		
3.53237	8.21813	11.2548	3.82535	36.6308	15.183	119.54	79.4133		
3.55039	8.11397	11.2645	3.81988	36.6345	15.2917	119.548	79.5464		
3.55158	8.10813	11.2723	3.82174	36.6465	15.1842	119.559	79.444		
3.83364	7.32071	12.2361	3.78188	39.8571	17.9589	130.08	86.1846		
3.84728	7.29769	12.2509	3.76598	39.8592	17.8141	130.093	86.2561		
3.84799	7.29475	12.2575	3.76276	39.8777	17.815	130.107	86.0954		
4.15481	6.89915	13.3164	3.76272	43.3696	20.9026	141.56	92.7334		
4.16878	6.88175	13.3275	3.74112	43.3702	20.729	141.563	92.9905		
4.16917	6.88167	13.3326	3.75334	43.3878	20.745	141.582	92.6062		
4.5068	6.54922	14.4868	3.83698	47.195	24.0023	154.038	99.2656		
4.52089	6.52994	14.4927	3.82958	47.2031	24.1507	154.045	98.8907		
4.52197	6.52685	14.4975	3.83031	47.2126	24.019	154.045	99.3724		
4.89	6.2242	15.7585	3.99106	51.3546	27.6085	167.64	106.488		
4.90399	6.21046	15.7708	3.99508	51.3576	27.8324	167.642	106.665		
4.90483	6.20422	15.7826	3.96766	51.3719	27.6199	167.666	106.488		
5.30785	5.91335	17.1377	4.25965	55.8798	31.5369	182.43	113.778		
5.32219	5.90454	17.1422	4.26761	55.8846	31.8146	182.436	113.873		
5.32286	5.89961	17.1577	4.29575	55.8973	31.544	182.454	113.703		
5.76346	5.60454	18.6462	4.6381	60.8125	35.7815	198.561	121.151		
5.77915	5.59038	18.6613	4.63894	60.8163	36.1283	198.565	121.126		
5.77978	5.58701	18.6794	4.57639	60.8337	35.7922	198.587	121.066		
6.26051	5.30689	20.2876	5.15371	66.1689	40.8174	215.991	128.669		
6.27711	5.2914	20.3095	5.18033	66.1696	40.3377	216.061	128.633		
6.27763	5.28838	20.3224	5.11405	66.1992	40.3544	216.067	128.68		
6.81131	5.00869	22.0746	5.85762	72.0012	45.8338	235.005	136.286		
6.82102	4.99896	22.0862	5.9169	72.0148	45.151	235.124	136.311		
6.84773	4.92124	22.1007	5.82975	72.0188	45.2184	235.124	136.282		

Table S10. Molar thermodynamic functions for krautite, $Mn[AsO_3(OH)]\cdot H_2O$, calculated from smoothed heat capacity.

T	C_p	H_T	$(H_T-H_0)/T$	S_T	G_T	$-(G_T-G_0)/T$
K	$J\cdot K^{-1}$	J	$J\cdot K^{-1}$	$J\cdot K^{-1}$	J	$J\cdot K^{-1}$
0	0	0	NaN	0	0	NaN
5	6.116	24.45	4.889	8.511	-18.11	3.621
10	3.988	48.51	4.851	11.93	-70.82	7.082
15	3.889	67.59	4.506	13.48	-134.6	8.976
20	5.05	89.47	4.474	14.73	-205.2	10.26
25	7.254	119.8	4.793	16.08	-282.1	11.29
30	10.3	163.4	5.447	17.66	-366.4	12.21
35	13.95	223.9	6.396	19.52	-459.2	13.12
40	17.97	303.5	7.588	21.64	-562	14.05
45	22.18	403.8	8.974	24	-676	15.02
50	26.49	525.5	10.51	26.56	-802.3	16.05
55	30.84	668.8	12.16	29.28	-941.8	17.12
60	35.2	833.9	13.9	32.15	-1095	18.26
65	39.51	1021	15.7	35.14	-1264	19.44
70	43.73	1229	17.56	38.23	-1447	20.67
75	47.77	1458	19.44	41.38	-1646	21.95
80	51.73	1706	21.33	44.59	-1861	23.26
85	55.59	1975	23.23	47.84	-2092	24.61
90	59.34	2262	25.14	51.13	-2339	25.99
95	62.98	2568	27.03	54.44	-2603	27.4
100	66.52	2892	28.92	57.76	-2884	28.84
110	73.3	3591	32.65	64.42	-3495	31.77
120	79.73	4357	36.31	71.07	-4172	34.77
130	85.86	5185	39.88	77.7	-4916	37.81
140	91.72	6073	43.38	84.28	-5726	40.9
150	97.32	7018	46.79	90.8	-6601	44.01
160	102.7	8019	50.12	97.25	-7542	47.14
170	107.8	9071	53.36	103.6	-8546	50.27
180	112.6	10170	56.52	109.9	-9614	53.41
190	117.3	11320	59.6	116.1	-10740	56.55
200	121.7	12520	62.59	122.3	-11940	59.68
210	126	13760	65.51	128.3	-13190	62.81
220	130.1	15040	68.36	134.3	-14500	65.92
230	134.2	16360	71.13	140.2	-15870	69.02
240	138.1	17720	73.84	145.9	-17310	72.11
250	141.9	19120	76.49	151.7	-18790	75.17
260	145.7	20560	79.08	157.3	-20340	78.22
270	149.3	22030	81.61	162.9	-21940	81.26
273.15	150.4	22510	82.4	164.6	-22460	82.21
280	152.8	23550	84.09	168.4	-23600	84.27
290	156.1	25090	86.52	173.8	-25310	87.26
298.15	158.6	26370	88.45	178.1	-26740	89.69
300	159.1	26670	88.89	179.1	-27070	90.24