Supporting information

Control the products selectivity and catalyst lifetime by acid strength, cavity size of SAPO, and diffusion rate of methanol in the MTO process:

DFT and MD calculation

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Computational details

Considering the ZPE and entropy corrections, the free energies of adsorption, ΔGads, can obtained by following equation:

$\Delta G_{ads} = \Delta E + \Delta ZPE - T\Delta S$

Detailed calculation:

(castep theoretical of material studio)

Thermodynamic calculations

The results of a calculation of phonon spectra can be used to compute energy (E), entropy (S), free energy (F), and lattice heat capacity (Cv) as functions of temperature. The CASTEP total energy yields the total electronic energy at 0 K. The vibrational contributions to the thermodynamic properties are evaluated to compute E, S, F, and Cv at finite temperatures as discussed below.

Thermodynamic calculations can be performed only if the system is in the ground state, that is, geometry optimization is fully converged. This means that all the phonon eigenfrequencies must be real and non-negative.

When you perform a vibrational analysis with CASTEP the results of the thermodynamic calculations can be visualized using the thermodynamic analysis tools.

The formulas below are based on work by Baroni et al. (2001).

The temperature dependence of the energy is given by:

$$E(T) = E_{tot} + E_{zp} + \int \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{kT}\right) - 1} F(\omega) d\omega$$

where Ezp if the zero point vibrational energy, k is the Boltzmann constant, ħ is the Planck constant and F(ω) is the phonon density of states. Ezp can be evaluated as:

$$E_{zp} = \frac{1}{2} \int F(w) \hbar\omega d\omega$$

The vibrational contribution to the free energy, F, is given by:

$$F(T) = E_{tot} + E_{zp} + kT \int F(\omega) \ln\left[1 - \exp\left(-\frac{\hbar\omega}{kT}\right)\right] d\omega$$

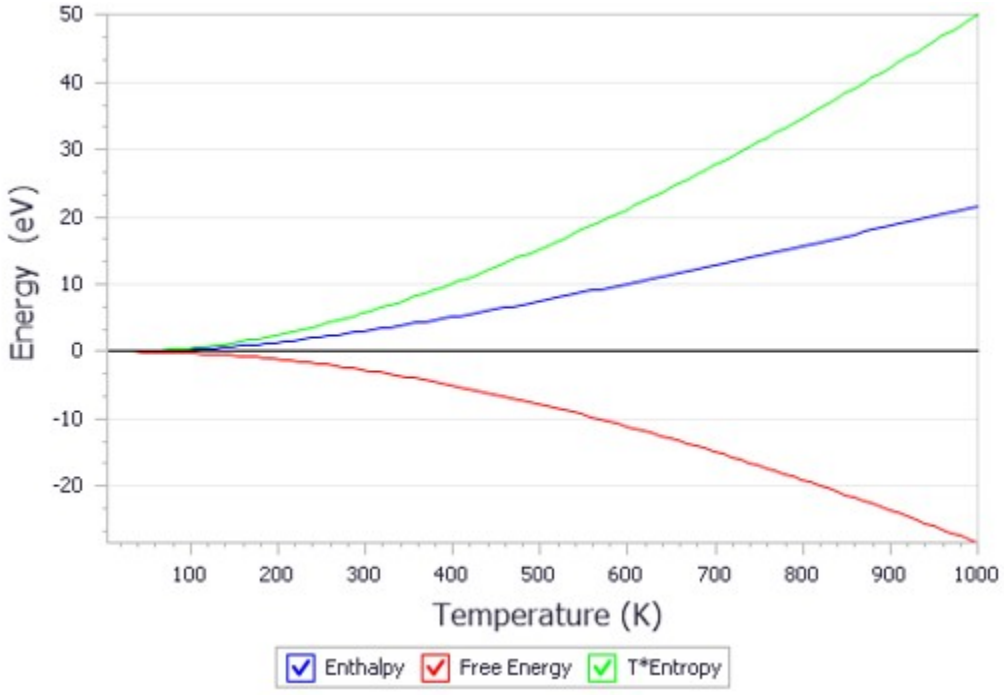

Fig 1s: Castep thermodynamic properties of SAPO-34 structure ($TS_{1\text{-}2}$).

Table 1S. Parameters of thermodynamic Castep of SAPO- 34 structure.

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
5	9.19E-05	5	-2.43E-05	5	0.000116
15.05051	0.002871	15.05051	-0.00142	15.05051	0.004292
25.10101	0.011259	25.10101	-0.00625	25.10101	0.01751
35.15152	0.027124	35.15152	-0.01582	35.15152	0.042941
45.20202	0.051347	45.20202	-0.03106	45.20202	0.082412
55.25253	0.084162	55.25253	-0.05263	55.25253	0.136796
65.30303	0.125495	65.30303	-0.08094	65.30303	0.206436
75.35354	0.175184	75.35354	-0.11625	75.35354	0.291432
85.40404	0.233061	85.40404	-0.15873	85.40404	0.391788
95.45455	0.29897	95.45455	-0.20849	95.45455	0.50746
105.5051	0.372751	105.5051	-0.26561	105.5051	0.638358
115.5556	0.454234	115.5556	-0.33012	115.5556	0.784355
125.6061	0.543233	125.6061	-0.40205	125.6061	0.945283
135.6566	0.639547	135.6566	-0.48139	135.6566	1.120941
145.7071	0.742961	145.7071	-0.56814	145.7071	1.3111
155.7576	0.853257	155.7576	-0.66226	155.7576	1.515513
165.8081	0.970213	165.8081	-0.76371	165.8081	1.733919
175.8586	1.093608	175.8586	-0.87244	175.8586	1.966051
185.9091	1.223227	185.9091	-0.98841	185.9091	2.211637
195.9596	1.35886	195.9596	-1.11155	195.9596	2.47041
206.0101	1.500304	206.0101	-1.2418	206.0101	2.7421
216.0606	1.647365	216.0606	-1.37908	216.0606	3.026447
226.1111	1.799856	226.1111	-1.52334	226.1111	3.323192
236.1616	1.957598	236.1616	-1.67449	236.1616	3.632083
246.2121	2.120416	246.2121	-1.83246	246.2121	3.952873
256.2626	2.288144	256.2626	-1.99718	256.2626	4.285321
266.3131	2.460622	266.3131	-2.16857	266.3131	4.62919
276.3636	2.637693	276.3636	-2.34656	276.3636	4.984251
286.4141	2.819207	286.4141	-2.53107	286.4141	5.350275
296.4646	3.005018	296.4646	-2.72202	296.4646	5.727041
306.5152	3.194983	306.5152	-2.91935	306.5152	6.114332
316.5657	3.388964	316.5657	-3.12297	316.5657	6.511935
326.6162	3.586828	326.6162	-3.33281	326.6162	6.919641
336.6667	3.788442	336.6667	-3.5488	336.6667	7.337246
346.7172	3.993682	346.7172	-3.77087	346.7172	7.764549
356.7677	4.202423	356.7677	-3.99893	356.7677	8.201354
366.8182	4.414546	366.8182	-4.23292	366.8182	8.64747
376.8687	4.629935	376.8687	-4.47277	376.8687	9.102709
386.9192	4.848477	386.9192	-4.71841	386.9192	9.566888

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
396.9697	5.070064	396.9697	-4.96976	396.9697	10.03983
407.0202	5.29459	407.0202	-5.22677	407.0202	10.52136
417.0707	5.521952	417.0707	-5.48935	417.0707	11.0113
427.1212	5.752053	427.1212	-5.75744	427.1212	11.50949
437.1717	5.984798	437.1717	-6.03098	437.1717	12.01578
447.2222	6.220093	447.2222	-6.3099	447.2222	12.52999
457.2727	6.457852	457.2727	-6.59414	457.2727	13.05199
467.3232	6.697988	467.3232	-6.88363	467.3232	13.58161
477.3737	6.940419	477.3737	-7.1783	477.3737	14.11872
487.4242	7.185067	487.4242	-7.47811	487.4242	14.66318
497.4747	7.431855	497.4747	-7.78298	497.4747	15.21484
507.5253	7.68071	507.5253	-8.09286	507.5253	15.77357
517.5758	7.931562	517.5758	-8.40769	517.5758	16.33925
527.6263	8.184343	527.6263	-8.72741	527.6263	16.91175
537.6768	8.438988	537.6768	-9.05196	537.6768	17.49095
547.7273	8.695435	547.7273	-9.38129	547.7273	18.07672
557.7778	8.953625	557.7778	-9.71534	557.7778	18.66896
567.8283	9.213499	567.8283	-10.0541	567.8283	19.26755
577.8788	9.475002	577.8788	-10.3974	577.8788	19.87239
587.9293	9.738083	587.9293	-10.7453	587.9293	20.48336
597.9798	10.00269	597.9798	-11.0977	597.9798	21.10037
608.0303	10.26877	608.0303	-11.4545	608.0303	21.72332
618.0808	10.53629	618.0808	-11.8158	618.0808	22.35211
628.1313	10.80518	628.1313	-12.1815	628.1313	22.98664
638.1818	11.07542	638.1818	-12.5514	638.1818	23.62684
648.2323	11.34697	648.2323	-12.9256	648.2323	24.27259
658.2828	11.61977	658.2828	-13.3041	658.2828	24.92383
668.3333	11.89379	668.3333	-13.6867	668.3333	25.58047
678.3838	12.169	678.3838	-14.0734	678.3838	26.24242
688.4343	12.44537	688.4343	-14.4642	688.4343	26.90961
698.4848	12.72285	698.4848	-14.8591	698.4848	27.58196
708.5354	13.00141	708.5354	-15.258	708.5354	28.25939
718.5859	13.28102	718.5859	-15.6608	718.5859	28.94184
728.6364	13.56166	728.6364	-16.0676	728.6364	29.62922
738.6869	13.8433	738.6869	-16.4782	738.6869	30.32148
748.7374	14.1259	748.7374	-16.8926	748.7374	31.01854
758.7879	14.40943	758.7879	-17.3109	758.7879	31.72035
768.8384	14.69389	768.8384	-17.7329	768.8384	32.42682

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
788.9394	15.26543	788.9394	-18.5881	788.9394	33.85356
798.9899	15.55248	798.9899	-19.0212	798.9899	34.57369
809.0404	15.84034	809.0404	-19.4579	809.0404	35.29826
819.0909	16.12901	819.0909	-19.8982	819.0909	36.02721
829.1414	16.41845	829.1414	-20.342	829.1414	36.76049
839.1919	16.70864	839.1919	-20.7894	839.1919	37.49803
879.3939	17.87663	879.3939	-22.6132	879.3939	40.48988
889.4444	18.17033	889.4444	-23.0777	889.4444	41.24801
899.4949	18.46469	899.4949	-23.5454	899.4949	42.01011
909.5455	18.75968	909.5455	-24.0165	909.5455	42.77615
919.596	19.0553	919.596	-24.4908	919.596	43.54606
929.6465	19.35151	929.6465	-24.9683	929.6465	44.31982
939.697	19.64832	939.697	-25.4491	939.697	45.09737
949.7475	19.94571	949.7475	-25.933	949.7475	45.87868
959.798	20.24366	959.798	-26.42	959.798	46.6637
969.8485	20.54216	969.8485	-26.9102	969.8485	47.4524
979.899	20.84119	979.899	-27.4035	979.899	48.24473
989.9495	21.14076	989.9495	-27.8999	989.9495	49.04065
1000	21.44084	1000	-28.3993	1000	49.84014

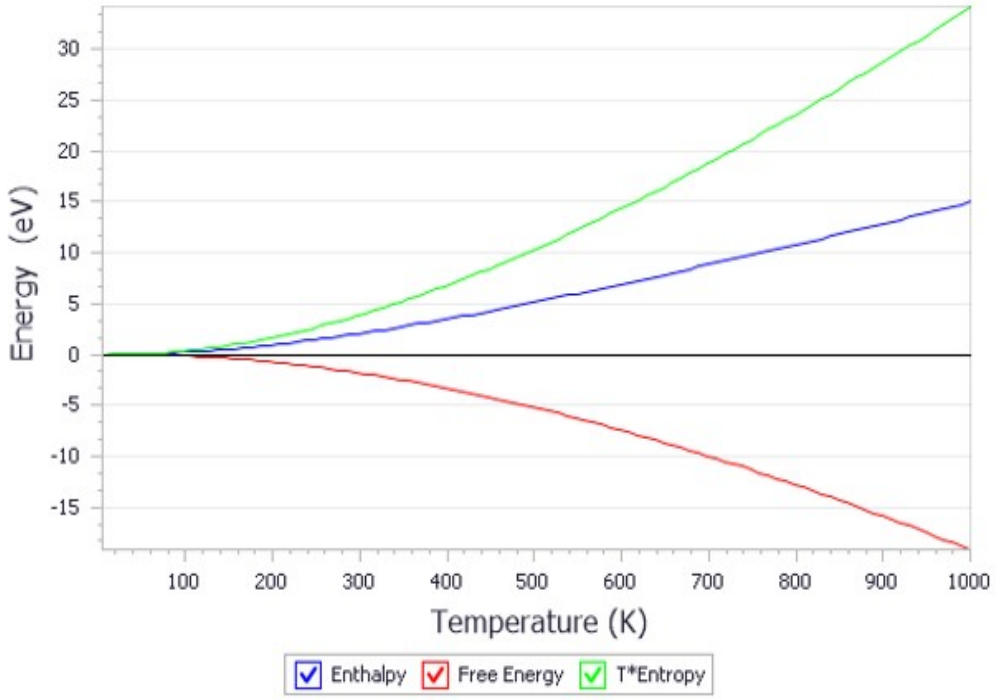

Fig 2S: Castep thermodynamic properties of SAPO-18 structure ($TS_{1\text{-}2}$).

Table 2S. Parameters of thermodynamic Castep of SAPO- 18 structure.

	T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
5	7.13E-05	5	-2.33E-05	5	9.45E-05	
15.05051	0.001441	15.05051	-0.0008	15.05051	0.002238	
25.10101	0.005935	25.10101	-0.00332	25.10101	0.009257	
35.15152	0.015124	35.15152	-0.00849	35.15152	0.023614	
45.20202	0.029836	45.20202	-0.01703	45.20202	0.046869	
55.25253	0.050348	55.25253	-0.02947	55.25253	0.079822	
65.30303	0.076688	65.30303	-0.04617	65.30303	0.122857	
75.35354	0.1088	75.35354	-0.06736	75.35354	0.176157	
85.40404	0.146605	85.40404	-0.09321	85.40404	0.239811	
95.45455	0.190015	95.45455	-0.12383	95.45455	0.313847	
105.5051	0.238931	105.5051	-0.15932	105.5051	0.39825	
115.5556	0.293239	115.5556	-0.19972	115.5556	0.492961	
125.6061	0.35281	125.6061	-0.24508	125.6061	0.597889	
135.6566	0.417506	135.6566	-0.29541	135.6566	0.712914	
145.7071	0.487177	145.7071	-0.35072	145.7071	0.837892	
155.7576	0.561671	155.7576	-0.411	155.7576	0.972667	
165.8081	0.640832	165.8081	-0.47623	165.8081	1.117067	
175.8586	0.72451	175.8586	-0.54641	175.8586	1.27092	
185.9091	0.812554	185.9091	-0.62149	185.9091	1.434048	
195.9596	0.904821	195.9596	-0.70145	195.9596	1.606272	
206.0101	1.001171	206.0101	-0.78625	206.0101	1.787419	
216.0606	1.101474	216.0606	-0.87584	216.0606	1.977315	
226.1111	1.2056	226.1111	-0.97019	226.1111	2.175791	
236.1616	1.313429	236.1616	-1.06925	236.1616	2.382681	
246.2121	1.424845	246.2121	-1.17298	246.2121	2.597824	
256.2626	1.539735	256.2626	-1.28133	256.2626	2.82106	
266.3131	1.657991	266.3131	-1.39424	266.3131	3.052235	
276.3636	1.779508	276.3636	-1.51169	276.3636	3.291197	
286.4141	1.904186	286.4141	-1.63361	286.4141	3.537797	
296.4646	2.031927	296.4646	-1.75996	296.4646	3.791888	
306.5152	2.162635	306.5152	-1.89069	306.5152	4.053328	
316.5657	2.296216	316.5657	-2.02576	316.5657	4.321975	
326.6162	2.432582	326.6162	-2.16511	326.6162	4.597692	
336.6667	2.571643	336.6667	-2.3087	336.6667	4.880342	
346.7172	2.713313	346.7172	-2.45648	346.7172	5.169793	
356.7677	2.85751	356.7677	-2.6084	356.7677	5.465915	
366.8182	3.004152	366.8182	-2.76443	366.8182	5.768577	
376.8687	3.15316	376.8687	-2.9245	376.8687	6.077657	
386.9192	3.304456	386.9192	-3.08857	386.9192	6.39303	
396.9697	3.457967	396.9697	-3.25661	396.9697	6.714576	

	T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
407.0202	3.613619	407.0202	-3.42856	407.0202	7.042178	
417.0707	3.771342	417.0707	-3.60438	417.0707	7.37572	
427.1212	3.931069	427.1212	-3.78402	427.1212	7.715091	
437.1717	4.092733	437.1717	-3.96745	437.1717	8.060181	
447.2222	4.256271	447.2222	-4.15461	447.2222	8.410883	
457.2727	4.42162	457.2727	-4.34547	457.2727	8.767092	
467.3232	4.588722	467.3232	-4.53999	467.3232	9.128708	
477.3737	4.757519	477.3737	-4.73811	477.3737	9.495632	
487.4242	4.927956	487.4242	-4.93981	487.4242	9.867766	
497.4747	5.09998	497.4747	-5.14504	497.4747	10.24502	
507.5253	5.273539	507.5253	-5.35376	507.5253	10.6273	
517.5758	5.448583	517.5758	-5.56593	517.5758	11.01451	
527.6263	5.625066	527.6263	-5.78151	527.6263	11.40658	
537.6768	5.802942	537.6768	-6.00047	537.6768	11.80342	
547.7273	5.982166	547.7273	-6.22277	547.7273	12.20494	
557.7778	6.162696	557.7778	-6.44837	557.7778	12.61107	
567.8283	6.344492	567.8283	-6.67723	567.8283	13.02172	
577.8788	6.527515	577.8788	-6.90932	577.8788	13.43684	
587.9293	6.711727	587.9293	-7.14461	587.9293	13.85634	
597.9798	6.897092	597.9798	-7.38305	597.9798	14.28015	
608.0303	7.083575	608.0303	-7.62462	608.0303	14.7082	
618.0808	7.271144	618.0808	-7.86929	618.0808	15.14043	
628.1313	7.459766	628.1313	-8.117	628.1313	15.57677	
638.1818	7.649411	638.1818	-8.36775	638.1818	16.01716	
648.2323	7.840049	648.2323	-8.62149	648.2323	16.46154	
658.2828	8.031652	658.2828	-8.8782	658.2828	16.90985	
668.3333	8.224193	668.3333	-9.13783	668.3333	17.36203	
678.3838	8.417645	678.3838	-9.40037	678.3838	17.81802	
688.4343	8.611983	688.4343	-9.66578	688.4343	18.27777	
698.4848	8.807183	698.4848	-9.93404	698.4848	18.74122	
708.5354	9.003222	708.5354	-10.2051	708.5354	19.20833	
718.5859	9.200077	718.5859	-10.479	718.5859	19.67904	
728.6364	9.397727	728.6364	-10.7556	728.6364	20.15331	
738.6869	9.596151	738.6869	-11.0349	738.6869	20.63108	
748.7374	9.79533	748.7374	-11.317	748.7374	21.11231	
758.7879	9.995242	758.7879	-11.6017	758.7879	21.59696	
768.8384	10.19587	768.8384	-11.8891	768.8384	22.08497	
778.8889	10.3972	778.8889	-12.1791	778.8889	22.57631	
788.9394	10.59921	788.9394	-12.4717	788.9394	23.07093	
798.9899	10.80188	798.9899	-12.7669	798.9899	23.56879	
809.0404	11.0052	809.0404	-13.0647	809.0404	24.06986	
819.0909	11.20915	819.0909	-13.3649	819.0909	24.57409	

	T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
839.1919	11.6189	839.1919	-13.973	839.1919	25.59188	
849.2424	11.82466	849.2424	-14.2807	849.2424	26.10537	
859.2929	12.031	859.2929	-14.5909	859.2929	26.62187	
869.3434	12.2379	869.3434	-14.9035	869.3434	27.14135	
879.3939	12.44535	879.3939	-15.2184	879.3939	27.66378	
889.4444	12.65334	889.4444	-15.5358	889.4444	28.18912	
899.4949	12.86185	899.4949	-15.8555	899.4949	28.71733	
909.5455	13.07088	909.5455	-16.1775	909.5455	29.2484	
919.596	13.28041	919.596	-16.5019	919.596	29.78228	
929.6465	13.49044	929.6465	-16.8285	929.6465	30.31894	
939.697	13.70094	939.697	-17.1574	939.697	30.85836	
949.7475	13.91192	949.7475	-17.4886	949.7475	31.40051	
959.798	14.12336	959.798	-17.822	959.798	31.94535	
969.8485	14.33525	969.8485	-18.1576	969.8485	32.49286	
979.899	14.54758	979.899	-18.4954	979.899	33.04301	
989.9495	14.76035	989.9495	-18.8354	989.9495	33.59577	
1000	14.97354	1000	-19.1776	1000	34.15113	

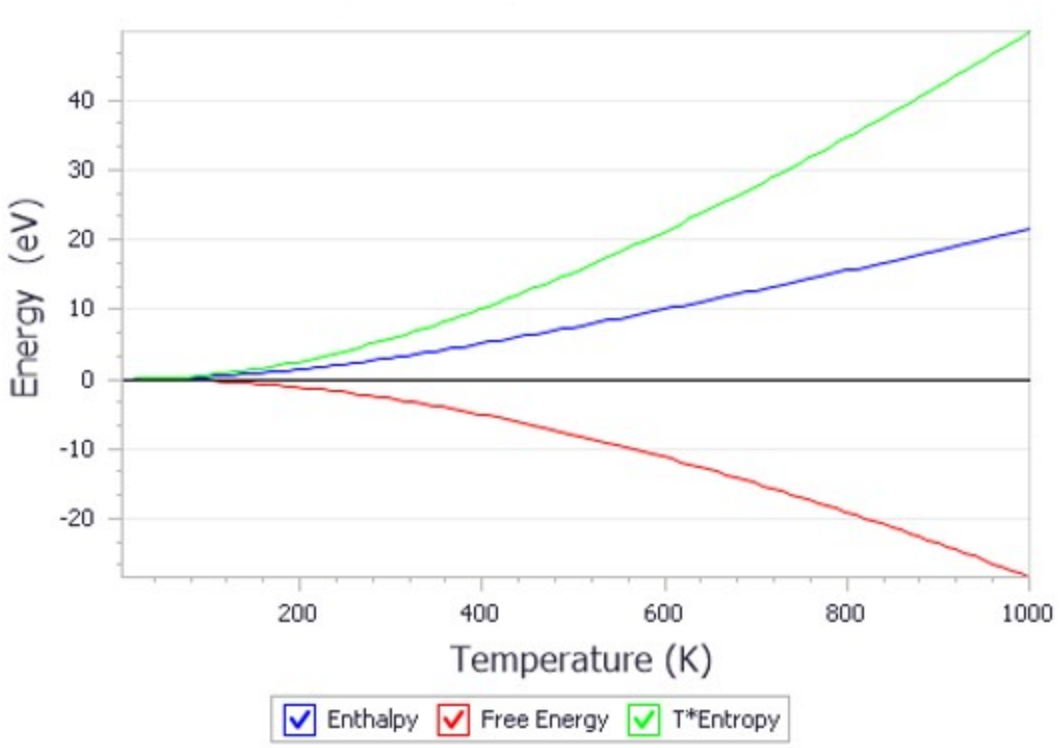

Fig 3S: Castep thermodynamic properties of SAPO-17 structure ($TS_{1\text{-}2}$).

Table 3S. Parameters of thermodynamic Castep of SAPO- 17 structure.

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
5	9.19E-05	5	-2.43E-05	5	0.000116
15.05051	0.002871	15.05051	-0.00142	15.05051	0.004292
25.10101	0.011259	25.10101	-0.00625	25.10101	0.01751
35.15152	0.027124	35.15152	-0.01582	35.15152	0.042941
45.20202	0.051347	45.20202	-0.03106	45.20202	0.082412
55.25253	0.084162	55.25253	-0.05263	55.25253	0.136796
65.30303	0.125495	65.30303	-0.08094	65.30303	0.206436
75.35354	0.175184	75.35354	-0.11625	75.35354	0.291432
85.40404	0.233061	85.40404	-0.15873	85.40404	0.391788
95.45455	0.29897	95.45455	-0.20849	95.45455	0.50746
105.5051	0.372751	105.5051	-0.26561	105.5051	0.638358
115.5556	0.454234	115.5556	-0.33012	115.5556	0.784355
125.6061	0.543233	125.6061	-0.40205	125.6061	0.945283
135.6566	0.639547	135.6566	-0.48139	135.6566	1.120941
145.7071	0.742961	145.7071	-0.56814	145.7071	1.3111
155.7576	0.853257	155.7576	-0.66226	155.7576	1.515513
165.8081	0.970213	165.8081	-0.76371	165.8081	1.733919
175.8586	1.093608	175.8586	-0.87244	175.8586	1.966051
185.9091	1.223227	185.9091	-0.98841	185.9091	2.211637
195.9596	1.35886	195.9596	-1.11155	195.9596	2.47041
206.0101	1.500304	206.0101	-1.2418	206.0101	2.7421
216.0606	1.647365	216.0606	-1.37908	216.0606	3.026447
226.1111	1.799856	226.1111	-1.52334	226.1111	3.323192
236.1616	1.957598	236.1616	-1.67449	236.1616	3.632083
246.2121	2.120416	246.2121	-1.83246	246.2121	3.952873
256.2626	2.288144	256.2626	-1.99718	256.2626	4.285321
266.3131	2.460622	266.3131	-2.16857	266.3131	4.62919
276.3636	2.637693	276.3636	-2.34656	276.3636	4.984251
286.4141	2.819207	286.4141	-2.53107	286.4141	5.350275
296.4646	3.005018	296.4646	-2.72202	296.4646	5.727041
306.5152	3.194983	306.5152	-2.91935	306.5152	6.114332
316.5657	3.388964	316.5657	-3.12297	316.5657	6.511935
326.6162	3.586828	326.6162	-3.33281	326.6162	6.919641
336.6667	3.788442	336.6667	-3.5488	336.6667	7.337246
346.7172	3.993682	346.7172	-3.77087	346.7172	7.764549
356.7677	4.202423	356.7677	-3.99893	356.7677	8.201354
366.8182	4.414546	366.8182	-4.23292	366.8182	8.64747
376.8687	4.629935	376.8687	-4.47277	376.8687	9.102709
386.9192	4.848477	386.9192	-4.71841	386.9192	9.566888

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
417.0707	5.521952	417.0707	-5.48935	417.0707	11.0113
427.1212	5.752053	427.1212	-5.75744	427.1212	11.50949
437.1717	5.984798	437.1717	-6.03098	437.1717	12.01578
447.2222	6.220093	447.2222	-6.3099	447.2222	12.52999
457.2727	6.457852	457.2727	-6.59414	457.2727	13.05199
467.3232	6.697988	467.3232	-6.88363	467.3232	13.58161
477.3737	6.940419	477.3737	-7.1783	477.3737	14.11872
487.4242	7.185067	487.4242	-7.47811	487.4242	14.66318
497.4747	7.431855	497.4747	-7.78298	497.4747	15.21484
507.5253	7.68071	507.5253	-8.09286	507.5253	15.77357
517.5758	7.931562	517.5758	-8.40769	517.5758	16.33925
527.6263	8.184343	527.6263	-8.72741	527.6263	16.91175
537.6768	8.438988	537.6768	-9.05196	537.6768	17.49095
547.7273	8.695435	547.7273	-9.38129	547.7273	18.07672
557.7778	8.953625	557.7778	-9.71534	557.7778	18.66896
567.8283	9.213499	567.8283	-10.0541	567.8283	19.26755
577.8788	9.475002	577.8788	-10.3974	577.8788	19.87239
587.9293	9.738083	587.9293	-10.7453	587.9293	20.48336
597.9798	10.00269	597.9798	-11.0977	597.9798	21.10037
608.0303	10.26877	608.0303	-11.4545	608.0303	21.72332
618.0808	10.53629	618.0808	-11.8158	618.0808	22.35211
628.1313	10.80518	628.1313	-12.1815	628.1313	22.98664
638.1818	11.07542	638.1818	-12.5514	638.1818	23.62684
648.2323	11.34697	648.2323	-12.9256	648.2323	24.27259
658.2828	11.61977	658.2828	-13.3041	658.2828	24.92383
668.3333	11.89379	668.3333	-13.6867	668.3333	25.58047
678.3838	12.169	678.3838	-14.0734	678.3838	26.24242
688.4343	12.44537	688.4343	-14.4642	688.4343	26.90961
698.4848	12.72285	698.4848	-14.8591	698.4848	27.58196
708.5354	13.00141	708.5354	-15.258	708.5354	28.25939
718.5859	13.28102	718.5859	-15.6608	718.5859	28.94184
728.6364	13.56166	728.6364	-16.0676	728.6364	29.62922
738.6869	13.8433	738.6869	-16.4782	738.6869	30.32148
748.7374	14.1259	748.7374	-16.8926	748.7374	31.01854
758.7879	14.40943	758.7879	-17.3109	758.7879	31.72035
768.8384	14.69389	768.8384	-17.7329	768.8384	32.42682
778.8889	14.97923	778.8889	-18.1587	778.8889	33.13791
788.9394	15.26543	788.9394	-18.5881	788.9394	33.85356
798.9899	15.55248	798.9899	-19.0212	798.9899	34.57369
809.0404	15.84034	809.0404	-19.4579	809.0404	35.29826
819.0909	16.12901	819.0909	-19.8982	819.0909	36.02721

T(K)	H(eV)	T(K)	G(eV)	T(K)	TS(eV.K)
839.1919	16.70864	839.1919	-20.7894	839.1919	37.49803
849.2424	16.99958	849.2424	-21.2402	849.2424	38.23979
859.2929	17.29123	859.2929	-21.6945	859.2929	38.98572
869.3434	17.58359	869.3434	-22.1522	869.3434	39.73576
879.3939	17.87663	879.3939	-22.6132	879.3939	40.48988
889.4444	18.17033	889.4444	-23.0777	889.4444	41.24801
899.4949	18.46469	899.4949	-23.5454	899.4949	42.01011
909.5455	18.75968	909.5455	-24.0165	909.5455	42.77615
919.596	19.0553	919.596	-24.4908	919.596	43.54606
929.6465	19.35151	929.6465	-24.9683	929.6465	44.31982
939.697	19.64832	939.697	-25.4491	939.697	45.09737
949.7475	19.94571	949.7475	-25.933	949.7475	45.87868
959.798	20.24366	959.798	-26.42	959.798	46.6637
969.8485	20.54216	969.8485	-26.9102	969.8485	47.4524
979.899	20.84119	979.899	-27.4035	979.899	48.24473
989.9495	21.14076	989.9495	-27.8999	989.9495	49.04065
1000	21.44084	1000	-28.3993	1000	49.84014