SUPPORTING INFORMATION

Thermodynamic Properties of Uranyl Containing Materials Based on Density Functional Theory

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Table S.1. Dehydrated schoepite bond distances (in Å).

Bond	Exp.^{1,2}	Exp.³	This work	DFT⁴
U-Oy	1.71	1.79	1.792	1.816
U-O	2.46	2.50	2.464	2.462
U-O'	2.51	2.51	2.518	2.536
O-O	2.49	2.64	2.521	2.534
O-O'	2.54	2.50	2.527	2.529
O-H	-	0.76	0.985	0.994
Oy-Oyd	3.06	2.87	2.999	2.995
Oy-Oye	3.13	3.21	3.099	3.070
Oy-O	2.88	2.76	2.806	2.763
Oy...HO	-	2.00	1.827	1.776

Table S.2. Dehydrated schoepite bond angles (in deg).

Angle	Exp.^{1,2}	Exp.³	This work	DFT⁴
Oy-U-Oy	180	180	180	180
O-H...Oy	-	178	172.310	171.8
O-U-O	-	63.6	60.791	61.9
O-U-O'	-	60.0	59.237	60.8
U-O-U	-	107.7	108.957	108.6
Oy-U-U-Oy	-	27.2	23.640	23.4

Table S.3. Main reflections in the X-Ray powder pattern of dehydrated schoepite.

This work			Exp.³	
2Θ (deg)	I (%)	hkl	2Θ	I (%)
17.187	72.958	020	17.201	72.747
25.729	27.126	002	25.925	25.080
26.135	100.0	111	26.141	100.0
31.107	30.321	022	31.280	30.517
34.776	9.778	040	34.806	26.043
36.055	34.754	131	36.074	36.193
42.708	12.059	200	42.591	12.139
43.760	13.111	042	43.908	13.498
45.615	29.579	113	45.858	28.215
46.357	12.121	220	46.253	12.130
50.962	20.421	151	50.998	20.431
52.399	18.087	133	52.628	18.259
53.770	13.907	222	53.783	14.122

Table S.4. Metastudtite bond distances (in Å). Atom numbering follows the same convention as in the work of Weck *et al.*⁵

Bond	This work	DFT ⁵
U1-O1	1.827	1.85
U1-O2	1.780	1.80
U1-O3	2.385	2.39
U1-O4	2.417	2.42
U1-U1	4.200	4.21
O3-O3'	1.428	1.46
O4-H1	0.983	1.00
O4-H2	0.995	1.00
O1...H2	1.818	1.75
O3...H1	1.705	1.67

Table S.5. Metastudtite bond angles (in deg). Atom numbering follows the same convention as in the work of Weck *et al.*⁵

Angle	This work	DFT ⁵
O1-U1-O2	179.68	178.8
O1-U1-O3	88.41	88.2
O1-U1-O4	88.00	88.4
O2-U1-O3	91.90	92.9
O2-U1-O4	92.01	91.7
O3-U1-O3'	34.83	35.5
O3-U1-O3'''	177.85	179.9
O3-U1-O3''''	145.09	144.5
O3-U1-O4	71.94	71.6
U1-O3-U1''	123.36	123.7
O4-U1-O3'	106.76	107.0
O4-U1-O4'	175.82	176.5
O1-U1-U1'-O1''	0.0	0.0

Table S.6. Main reflections in the X-Ray powder spectrum of metastudtite.

This work			Exp. ⁶	
2 Θ (deg)	I (%)	hkl	2 Θ	I (%)
16.594	100.00	011	16.939	100
20.715	31.726	020	20.211	33
23.577	29.755	210	23.390	33
24.878	36.498	201	25.208	34
26.095	15.134	002	27.420	15
32.589	20.496	221	32.533	21
33.998	18.811	031	33.575	21
33.549	8.074	022	34.317	9
35.453	19.618	212	36.357	19
38.073	14.559	230	37.408	15
42.149	5.4580	040	41.127	13
41.020	6.999	013	42.930	12
46.742	10.965	232	46.458	13
45.305	8.830	203	46.993	13
49.564	11.705	241	48.845	13

Table S.7. Calculated isobaric heat capacity function of dehydrated schoepite. Temperature and heat capacity values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	C _p	T	C _p	T	C _p
15.05051	2.87289	346.71717	111.4699	678.38384	137.28562
25.10101	7.79176	356.76768	112.86234	688.43434	137.6959
35.15152	13.1956	366.81818	114.19619	698.48485	138.09548
45.20202	18.81279	376.86869	115.47375	708.53535	138.48487
55.25253	24.57121	386.91919	116.69736	718.58586	138.86458
65.30303	30.34143	396.9697	117.86931	728.63636	139.23505
75.35354	35.98446	407.0202	118.99189	738.68687	139.59672
85.40404	41.39041	417.07071	120.06733	748.73737	139.95
95.45455	46.48963	427.12121	121.09783	758.78788	140.29526
105.50505	51.25007	437.17172	122.08552	768.83838	140.63286
115.55556	55.66932	447.22222	123.03249	778.88889	140.96313
125.60606	59.7652	457.27273	123.94073	788.93939	141.28639
135.65657	63.56715	467.32323	124.8122	798.9899	141.60293
145.70707	67.10933	477.37374	125.64875	809.0404	141.91301
155.75758	70.42581	487.42424	126.45219	819.09091	142.21692
165.80808	73.5477	497.47475	127.22423	829.14141	142.51487
175.85859	76.50171	507.52525	127.96652	839.19192	142.80711
185.90909	79.30976	517.57576	128.68062	849.24242	143.09384
195.9596	81.98928	527.62626	129.36803	859.29293	143.37526
206.0101	84.55373	537.67677	130.03017	869.34343	143.65158
216.06061	87.01332	547.72727	130.66838	879.39394	143.92295
226.11111	89.37574	557.77778	131.28395	889.44444	144.18956
236.16162	91.64676	567.82828	131.87809	899.49495	144.45155
246.21212	93.83078	577.87879	132.45195	909.54545	144.70907
256.26263	95.93124	587.92929	133.00661	919.59596	144.96227
266.31313	97.95096	597.9798	133.54309	929.64646	145.21128
276.36364	99.89236	608.0303	134.06236	939.69697	145.45622
286.41414	101.75766	618.08081	134.56534	949.74747	145.6972
296.46465	103.54897	628.13131	135.05287	959.79798	145.93435
306.51515	105.26839	638.18182	135.52577	969.84848	146.16776
316.56566	106.91801	648.23232	135.98481	979.89899	146.39754
326.61616	108.5	658.28283	136.43069	989.94949	146.62377
336.66667	110.01654	668.33333	136.86408	1000	146.84656

Table S.8. Calculated entropy function of dehydrated schoepite. Temperature and entropy values are given in K and J·K⁻¹·mol⁻¹ units, respectively.

T	S	T	S	T	S
15.05051	1.25854	346.71717	142.17733	678.38384	230.3699
25.10101	3.9592	356.76768	145.53012	688.43434	232.4849
35.15152	7.59635	366.81818	148.8294	698.48485	234.57529
45.20202	11.76663	376.86869	152.07623	708.53535	236.64213
55.25253	16.30135	386.91919	155.27221	718.58586	238.68505
65.30303	21.08764	396.9697	158.41816	728.63636	240.70538
75.35354	26.04725	407.0202	161.51542	738.68687	242.70306
85.40404	31.1077	417.07071	164.56519	748.73737	244.679
95.45455	36.21944	427.12121	167.56858	758.78788	246.63312
105.50505	41.33581	437.17172	170.52656	768.83838	248.56658
115.55556	46.42429	447.22222	173.44059	778.88889	250.47925
125.60606	51.45892	457.27273	176.31145	788.93939	252.37194
135.65657	56.42323	467.32323	179.13986	798.9899	254.24477
145.70707	61.30858	477.37374	181.92699	809.0404	256.09822
155.75758	66.1055	487.42424	184.67441	819.09091	257.93297
165.80808	70.81405	497.47475	187.38208	829.14141	259.74914
175.85859	75.43292	507.52525	190.05191	839.19192	261.54709
185.90909	79.9611	517.57576	192.68376	849.24242	263.3272
195.9596	84.40268	527.62626	195.27935	859.29293	265.08981
206.0101	88.75981	537.67677	197.83936	869.34343	266.83553
216.06061	93.0331	547.72727	200.36444	879.39394	268.56439
226.11111	97.22734	557.77778	202.8556	889.44444	270.27668
236.16162	101.34547	567.82828	205.3138	899.49495	271.97297
246.21212	105.38799	577.87879	207.73909	909.54545	273.65325
256.26263	109.35908	587.92929	210.13315	919.59596	275.31831
266.31313	113.25961	597.9798	212.49595	929.64646	276.96787
276.36364	117.09288	608.0303	214.82864	939.69697	278.60267
286.41414	120.8601	618.08081	217.13229	949.74747	280.22244
296.46465	124.56309	628.13131	219.40678	959.79798	281.82813
306.51515	128.20425	638.18182	221.65309	969.84848	283.41945
316.56566	131.78488	648.23232	223.87179	979.89899	284.99707
326.61616	135.30615	658.28283	226.06378	989.94949	286.56094
336.66667	138.76979	668.33333	228.22955	1000	288.11123

Table S.9. Calculated enthalpy function, ΔH ($\Delta H = H_T - H_{298}$), of dehydrated schoepite. Temperature and enthalpy values are given in K and $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ units, respectively.

T	$H_T - H_{298}$	T	$H_T - H_{298}$	T	$H_T - H_{298}$
15.05051	-1264.62678	346.71717	15.79245	678.38384	73.03877
25.10101	-756.06396	356.76768	18.65305	688.43434	74.07195
35.15152	-536.76131	366.81818	21.39569	698.48485	75.08161
45.20202	-413.69501	376.86869	24.02853	708.53535	76.06841
55.25253	-334.31779	386.91919	26.55888	718.58586	77.03332
65.30303	-278.44299	396.9697	28.9927	728.63636	77.9769
75.35354	-236.67603	407.0202	31.33536	738.68687	78.90036
85.40404	-204.05885	417.07071	33.59346	748.73737	79.80354
95.45455	-177.73155	427.12121	35.77126	758.78788	80.68787
105.50505	-155.92864	437.17172	37.87266	768.83838	81.55379
115.55556	-137.49879	447.22222	39.90279	778.88889	82.40201
125.60606	-121.66497	457.27273	41.86479	788.93939	83.2326
135.65657	-107.86971	467.32323	43.76252	798.9899	84.04681
145.70707	-95.71436	477.37374	45.59904	809.0404	84.84468
155.75758	-84.8954	487.42424	47.37715	819.09091	85.62708
165.80808	-75.18436	497.47475	49.10086	829.14141	86.3943
175.85859	-66.40088	507.52525	50.77152	839.19192	87.14659
185.90909	-58.40492	517.57576	52.3922	849.24242	87.88505
195.9596	-51.08267	527.62626	53.96486	859.29293	88.60933
206.0101	-44.34023	537.67677	55.49218	869.34343	89.32046
216.06061	-38.10338	547.72727	56.97578	879.39394	90.01864
226.11111	-32.30896	557.77778	58.41759	889.44444	90.70401
236.16162	-26.90458	567.82828	59.81983	899.49495	91.37729
246.21212	-21.84638	577.87879	61.18373	909.54545	92.03861
256.26263	-17.09647	587.92929	62.51126	919.59596	92.68862
266.31313	-12.62446	597.9798	63.80384	929.64646	93.32717
276.36364	-8.40266	608.0303	65.06242	939.69697	93.95488
286.41414	-4.4064	618.08081	66.28904	949.74747	94.5721
296.46465	-0.61683	628.13131	67.48486	959.79798	95.17891
306.51515	2.98482	638.18182	68.65057	969.84848	95.77563
316.56566	6.41341	648.23232	69.78795	979.89899	96.36281
326.61616	9.68342	658.28283	70.89756	989.94949	96.94027
336.66667	12.80619	668.33333	71.98102	1000	97.50877

Table S.10. Calculated free-energy function, ΔG ($\Delta G = G_T - G_{298}$), of dehydrated schoepite. Temperature and free-energy values are given in K and J·K⁻¹·mol⁻¹ units, respectively.

T	G _T -G ₂₉₈	T	G _T -G ₂₉₈	T	G _T -G ₂₉₈
15.05051	-1265.88532	346.71717	-126.38487	678.38384	-157.33113
25.10101	-760.02316	356.76768	-126.87707	688.43434	-158.41295
35.15152	-544.35079	366.81818	-127.4337	698.48485	-159.49368
45.20202	-425.46164	376.86869	-128.04769	708.53535	-160.57337
55.25253	-350.61913	386.91919	-128.71332	718.58586	-161.65173
65.30303	-299.53063	396.9697	-129.42545	728.63636	-162.72815
75.35354	-262.72328	407.0202	-130.18006	738.68687	-163.8027
85.40404	-235.16655	417.07071	-130.97173	748.73737	-164.87515
95.45455	-213.95099	427.12121	-131.79788	758.78788	-165.94525
105.50505	-197.26446	437.17172	-132.6539	768.83838	-167.01279
115.55556	-183.92308	447.22222	-133.5378	778.88889	-168.07724
125.60606	-173.12197	457.27273	-134.44666	788.93939	-169.13903
135.65657	-164.29293	467.32323	-135.37734	798.9899	-170.19796
145.70707	-157.02129	477.37374	-136.32846	809.0404	-171.25354
155.75758	-151.00089	487.42424	-137.29676	819.09091	-172.30589
165.80808	-145.9984	497.47475	-138.2817	829.14141	-173.35483
175.85859	-141.8338	507.52525	-139.28039	839.19192	-174.4005
185.90909	-138.36731	517.57576	-140.29203	849.24242	-175.44215
195.9596	-135.48535	527.62626	-141.31449	859.29293	-176.48049
206.0101	-133.10004	537.67677	-142.34719	869.34343	-177.51507
216.06061	-131.1376	547.72727	-143.38866	879.39394	-178.54575
226.11111	-129.53737	557.77778	-144.43801	889.44444	-179.57267
236.16162	-128.25004	567.82828	-145.49397	899.49495	-180.59568
246.21212	-127.23437	577.87879	-146.55536	909.54545	-181.61464
256.26263	-126.45555	587.92929	-147.62189	919.59596	-182.62969
266.31313	-125.88407	597.9798	-148.69211	929.64646	-183.6407
276.36364	-125.49467	608.0303	-149.76622	939.69697	-184.64754
286.41414	-125.2665	618.08081	-150.84286	949.74747	-185.65034
296.46465	-125.17992	628.13131	-151.92192	959.79798	-186.64922
306.51515	-125.21943	638.18182	-153.00251	969.84848	-187.64382
316.56566	-125.37148	648.23232	-154.08421	979.89899	-188.63426
326.61616	-125.62347	658.28283	-155.16622	989.94949	-189.62043
336.66667	-125.96431	668.33333	-156.24889	1000	-190.6027

Table S.11. Calculated isobaric heat capacity function of metastudtite. Temperature and heat capacity values are given in K and J·K⁻¹·mol⁻¹ units, respectively.

T	Cp	T	Cp	T	Cp
15.05051	3.20031	346.71717	174.80111	678.38384	215.68113
25.10101	10.4237	356.76768	176.90778	688.43434	216.41476
35.15152	18.39577	366.81818	178.9236	698.48485	217.1336
45.20202	26.67115	376.86869	180.85382	708.53535	217.83824
55.25253	35.15641	386.91919	182.70339	718.58586	218.52932
65.30303	43.6934	396.9697	184.47697	728.63636	219.20736
75.35354	52.12303	407.0202	186.17898	738.68687	219.87289
85.40404	60.32173	417.07071	187.81355	748.73737	220.5264
95.45455	68.20558	427.12121	189.38454	758.78788	221.16833
105.50505	75.72558	437.17172	190.89563	768.83838	221.79911
115.55556	82.86075	447.22222	192.35025	778.88889	222.41913
125.60606	89.61057	457.27273	193.75162	788.93939	223.02877
135.65657	95.98769	467.32323	195.10278	798.9899	223.62836
145.70707	102.01201	477.37374	196.40657	809.0404	224.21823
155.75758	107.70632	487.42424	197.66568	819.09091	224.79868
165.80808	113.09355	497.47475	198.88262	829.14141	225.37002
175.85859	118.19531	507.52525	200.05976	839.19192	225.93249
185.90909	123.03125	517.57576	201.19931	849.24242	226.48635
195.9596	127.61899	527.62626	202.30335	859.29293	227.03184
206.0101	131.97421	537.67677	203.37382	869.34343	227.56919
216.06061	136.11102	547.72727	204.41257	879.39394	228.09859
226.11111	140.04222	557.77778	205.42131	889.44444	228.62026
236.16162	143.77955	567.82828	206.40166	899.49495	229.13438
246.21212	147.33387	577.87879	207.35511	909.54545	229.64111
256.26263	150.71537	587.92929	208.28308	919.59596	230.14064
266.31313	153.93363	597.9798	209.18689	929.64646	230.63312
276.36364	156.99773	608.0303	210.0678	939.69697	231.11869
286.41414	159.91628	618.08081	210.92696	949.74747	231.59751
296.46465	162.69745	628.13131	211.76543	959.79798	232.06971
306.51515	165.34903	638.18182	212.58426	969.84848	232.53542
316.56566	167.87839	648.23232	213.38439	979.89899	232.99477
326.61616	170.29249	658.28283	214.16669	989.94949	233.44788
336.66667	172.59798	668.33333	214.93202	1000	233.89485

Table S.12. Calculated entropy function of metastudtite. Temperature and entropy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	S	T	S	T	S
15.05051	0.90369	346.71717	204.77768	678.38384	336.76621
25.10101	4.161	356.76768	209.80294	688.43434	339.94351
35.15152	8.93446	366.81818	214.7455	698.48485	343.08531
45.20202	14.54686	376.86869	219.60813	708.53535	346.19245
55.25253	20.72375	386.91919	224.3927	718.58586	349.26571
65.30303	27.29315	396.9697	229.10088	728.63636	352.3055
75.35354	34.13961	407.0202	233.73419	738.68687	355.31318
85.40404	41.17096	417.07071	238.29571	748.73737	358.28877
95.45455	48.31618	427.12121	242.78714	758.78788	361.23385
105.50505	55.51756	437.17172	247.20944	768.83838	364.14805
115.55556	62.73123	447.22222	251.56458	778.88889	367.03288
125.60606	69.9216	457.27273	255.8554	788.93939	369.88823
135.65657	77.06361	467.32323	260.08245	798.9899	372.71553
145.70707	84.13914	477.37374	264.24772	809.0404	375.51461
155.75758	91.13316	487.42424	268.35306	819.09091	378.28653
165.80808	98.03724	497.47475	272.39967	829.14141	381.0314
175.85859	104.84209	507.52525	276.38963	839.19192	383.75018
185.90909	111.54565	517.57576	280.32389	849.24242	386.44324
195.9596	118.14381	527.62626	284.20428	859.29293	389.1112
206.0101	124.63561	537.67677	288.03156	869.34343	391.75438
216.06061	131.02136	547.72727	291.80779	879.39394	394.37334
226.11111	137.29922	557.77778	295.53356	889.44444	396.96837
236.16162	143.47069	567.82828	299.21112	899.49495	399.54
246.21212	149.53706	577.87879	302.84048	909.54545	402.08902
256.26263	155.49939	587.92929	306.42413	919.59596	404.61536
266.31313	161.3595	597.9798	309.96233	929.64646	407.11951
276.36364	167.11894	608.0303	313.45617	939.69697	409.60218
286.41414	172.77904	618.08081	316.90701	949.74747	412.06355
296.46465	178.34259	628.13131	320.31617	959.79798	414.50403
306.51515	183.81121	638.18182	323.68447	969.84848	416.92403
316.56566	189.18708	648.23232	327.01233	979.89899	419.32367
326.61616	194.47213	658.28283	330.30158	989.94949	421.70358
336.66667	199.66803	668.33333	333.55219	1000	424.06388

Table S.13. Calculated enthalpy function, ΔH ($\Delta H = H_T - H_{298}$), of metastudtite. Temperature and enthalpy values are given in K and $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ units, respectively.

T	$H_T - H_{298}$	T	$H_T - H_{298}$	T	$H_T - H_{298}$
15.05051	-1857.91427	346.71717	23.70007	678.38384	109.35331
25.10101	-1111.32211	356.76768	27.98626	688.43434	110.91097
35.15152	-789.46289	366.81818	32.09478	698.48485	112.43416
45.20202	-608.92329	376.86869	36.036	708.53535	113.92436
55.25253	-492.54072	386.91919	39.82235	718.58586	115.3826
65.30303	-410.66713	396.9697	43.46255	728.63636	116.80988
75.35354	-349.50056	407.0202	46.96564	738.68687	118.2078
85.40404	-301.75037	417.07071	50.3398	748.73737	119.57688
95.45455	-263.21146	427.12121	53.59357	758.78788	120.91828
105.50505	-231.27889	437.17172	56.73305	768.83838	122.23277
115.55556	-204.26435	447.22222	59.76432	778.88889	123.52169
125.60606	-181.0161	457.27273	62.69399	788.93939	124.78542
135.65657	-160.72724	467.32323	65.52707	798.9899	126.0249
145.70707	-142.81023	477.37374	68.26915	809.0404	127.24134
155.75758	-126.82759	487.42424	70.92438	819.09091	128.4347
165.80808	-112.44648	497.47475	73.49704	829.14141	129.6064
175.85859	-99.40878	507.52525	75.99206	839.19192	130.75664
185.90909	-87.51347	517.57576	78.41208	849.24242	131.8862
195.9596	-76.59585	527.62626	80.76185	859.29293	132.99579
206.0101	-66.52571	537.67677	83.04351	869.34343	134.0861
216.06061	-57.19595	547.72727	85.26125	879.39394	135.15752
226.11111	-48.51531	557.77778	87.41724	889.44444	136.2107
236.16162	-40.4101	567.82828	89.51474	899.49495	137.24625
246.21212	-32.81868	577.87879	91.55598	909.54545	138.26421
256.26263	-25.68623	587.92929	93.54344	919.59596	139.26569
266.31313	-18.96714	597.9798	95.47941	929.64646	140.25096
276.36364	-12.62329	608.0303	97.36646	939.69697	141.22004
286.41414	-6.61939	618.08081	99.20619	949.74747	142.17394
296.46465	-0.92656	628.13131	101.00048	959.79798	143.11289
306.51515	4.48265	638.18182	102.75111	969.84848	144.0371
316.56566	9.63068	648.23232	104.46048	979.89899	144.94728
326.61616	14.53722	658.28283	106.12938	989.94949	145.84336
336.66667	19.22174	668.33333	107.75999	1000	146.72625

Table S.14. Calculated free-energy function, ΔG ($\Delta G = G_T - G_{298}$), of metastudtite. Temperature and free-energy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	$G_T - G_{298}$	T	$G_T - G_{298}$	T	$G_T - G_{298}$
15.05051	-1858.81796	346.71717	-181.0776	678.38384	-227.41291
25.10101	-1115.49273	356.76768	-181.81668	688.43434	-229.03254
35.15152	-798.39735	366.81818	-182.65138	698.48485	-230.65115
45.20202	-623.47549	376.86869	-183.57212	708.53535	-232.26809
55.25253	-513.26447	386.91919	-184.57035	718.58586	-233.88311
65.30303	-437.96027	396.9697	-185.63833	728.63636	-235.49562
75.35354	-383.64017	407.0202	-186.76914	738.68687	-237.10539
85.40404	-342.92416	417.07071	-187.95591	748.73737	-238.71221
95.45455	-311.52763	427.12121	-189.19357	758.78788	-240.31557
105.50505	-286.79646	437.17172	-190.47639	768.83838	-241.91529
115.55556	-266.9935	447.22222	-191.80026	778.88889	-243.51119
125.60606	-250.93771	457.27273	-193.16141	788.93939	-245.10282
135.65657	-237.79263	467.32323	-194.55538	798.9899	-246.69032
145.70707	-226.94937	477.37374	-195.97857	809.0404	-248.27328
155.75758	-217.96075	487.42424	-197.42868	819.09091	-249.85183
165.80808	-210.48226	497.47475	-198.90263	829.14141	-251.42529
175.85859	-204.25086	507.52525	-200.39757	839.19192	-252.99382
185.90909	-199.05912	517.57576	-201.91181	849.24242	-254.55704
195.9596	-194.73966	527.62626	-203.44243	859.29293	-256.11541
206.0101	-191.16249	537.67677	-204.98805	869.34343	-257.66828
216.06061	-188.21619	547.72727	-206.54654	879.39394	-259.21554
226.11111	-185.81346	557.77778	-208.11632	889.44444	-260.75767
236.16162	-183.88079	567.82828	-209.69638	899.49495	-262.29403
246.21212	-182.35574	577.87879	-211.28491	909.54545	-263.82454
256.26263	-181.18562	587.92929	-212.88069	919.59596	-265.34967
266.31313	-180.32755	597.9798	-214.48252	929.64646	-266.86881
276.36364	-179.74223	608.0303	-216.08971	939.69697	-268.38215
286.41414	-179.39928	618.08081	-217.70122	949.74747	-269.88962
296.46465	-179.26915	628.13131	-219.31569	959.79798	-271.39114
306.51515	-179.32856	638.18182	-220.93298	969.84848	-272.88668
316.56566	-179.5564	648.23232	-222.55185	979.89899	-274.37639
326.61616	-179.93491	658.28283	-224.17184	989.94949	-275.85998
336.66667	-180.44629	668.33333	-225.79256	1000	-277.33787

Table S.15. Calculated isobaric heat capacity function of studtite. Temperature and heat capacity values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	C _p	T	C _p	T	C _p
15.05051	4.04792	346.71717	238.51119	678.38384	310.2368
25.10101	11.39871	356.76768	241.9512	688.43434	311.62229
35.15152	20.3352	366.81818	245.2677	698.48485	312.98285
45.20202	31.05617	376.86869	248.4663	708.53535	314.31943
55.25253	42.87541	386.91919	251.55246	718.58586	315.63293
65.30303	54.98831	396.9697	254.53143	728.63636	316.92416
75.35354	66.86329	407.0202	257.40836	738.68687	318.19391
85.40404	78.22091	417.07071	260.18814	748.73737	319.44292
95.45455	88.94408	427.12121	262.8755	758.78788	320.67184
105.50505	99.01028	437.17172	265.475	768.83838	321.88134
115.55556	108.44851	447.22222	267.99098	778.88889	323.072
125.60606	117.31252	457.27273	270.42761	788.93939	324.24438
135.65657	125.66446	467.32323	272.78886	798.9899	325.39901
145.70707	133.56515	477.37374	275.07852	809.0404	326.53637
155.75758	141.06906	487.42424	277.30022	819.09091	327.65694
165.80808	148.22223	497.47475	279.45736	829.14141	328.76113
175.85859	155.06205	507.52525	281.55323	839.19192	329.84936
185.90909	161.6182	517.57576	283.59091	849.24242	330.92203
195.9596	167.91379	527.62626	285.57332	859.29293	331.97947
206.0101	173.96682	537.67677	287.50326	869.34343	333.02204
216.06061	179.79141	547.72727	289.38332	879.39394	334.05007
226.11111	185.39893	557.77778	291.21598	889.44444	335.06385
236.16162	190.79881	567.82828	293.00358	899.49495	336.06368
246.21212	195.9992	577.87879	294.74831	909.54545	337.04984
256.26263	201.00745	587.92929	296.45225	919.59596	338.02259
266.31313	205.83041	597.9798	298.11734	929.64646	338.98216
276.36364	210.47465	608.0303	299.7454	939.69697	339.92881
286.41414	214.94661	618.08081	301.33815	949.74747	340.86277
296.46465	219.25261	628.13131	302.89722	959.79798	341.78424
306.51515	223.39894	638.18182	304.42411	969.84848	342.69345
316.56566	227.39183	648.23232	305.92022	979.89899	343.59058
326.61616	231.23745	658.28283	307.38689	989.94949	344.47584
336.66667	234.9419	668.33333	308.82537	1000	345.34941

Table S.16. Calculated entropy function of studtite. Temperature and entropy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	S	T	S	T	S
15.05051	1.41923	346.71717	266.72128	678.38384	451.93623
25.10101	5.1508	356.76768	273.58557	688.43434	456.50918
35.15152	10.35491	366.81818	280.35385	698.48485	461.03548
45.20202	16.72942	376.86869	287.02674	708.53535	465.51645
55.25253	24.0984	386.91919	293.60671	718.58586	469.95296
65.30303	32.25017	396.9697	300.09593	728.63636	474.34587
75.35354	40.95472	407.0202	306.4958	738.68687	478.6963
85.40404	50.03104	417.07071	312.80874	748.73737	483.00501
95.45455	59.32377	427.12121	319.03636	758.78788	487.27237
105.50505	68.72993	437.17172	325.18068	768.83838	491.50001
115.55556	78.16564	447.22222	331.24355	778.88889	495.68822
125.60606	87.57772	457.27273	337.22663	788.93939	499.83791
135.65657	96.92874	467.32323	343.13148	798.9899	503.94961
145.70707	106.19162	477.37374	348.96049	809.0404	508.02446
155.75758	115.35088	487.42424	354.71491	819.09091	512.0629
165.80808	124.39484	497.47475	360.39682	829.14141	516.06571
175.85859	133.31855	507.52525	366.00721	839.19192	520.03328
185.90909	142.11817	517.57576	371.54837	849.24242	523.9666
195.9596	150.7931	527.62626	377.02153	859.29293	527.86629
206.0101	159.34286	537.67677	382.42869	869.34343	531.73269
216.06061	167.76816	547.72727	387.77042	879.39394	535.56667
226.11111	176.06961	557.77778	393.04894	889.44444	539.36851
236.16162	184.24972	567.82828	398.2655	899.49495	543.13903
246.21212	192.31064	577.87879	403.42166	909.54545	546.87873
256.26263	200.25226	587.92929	408.51887	919.59596	550.58809
266.31313	208.07813	597.9798	413.55768	929.64646	554.2676
276.36364	215.78864	608.0303	418.5402	939.69697	557.91793
286.41414	223.3867	618.08081	423.46761	949.74747	561.53926
296.46465	230.87478	628.13131	428.34064	959.79798	565.13224
306.51515	238.25347	638.18182	433.16109	969.84848	568.69727
316.56566	245.52557	648.23232	437.92957	979.89899	572.23495
326.61616	252.6928	658.28283	442.64771	989.94949	575.74564
336.66667	259.75737	668.33333	447.31634	1000	579.22966

Table S.17. Calculated enthalpy function, ΔH ($\Delta H = H_T - H_{298}$), of studtite. Temperature and enthalpy values are given in K and $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ units, respectively.

T(K)	$H_T - H_{298}$	T	$H_T - H_{298}$	T	$H_T - H_{298}$
15.05051	-2443.72993	346.71717	32.14957	678.38384	153.28092
25.10101	-1462.20898	356.76768	38.01172	688.43434	155.58233
35.15152	-1039.6469	366.81818	43.64535	698.48485	157.83754
45.20202	-802.79676	376.86869	49.06555	708.53535	160.04783
55.25253	-650.05257	386.91919	54.28521	718.58586	162.21476
65.30303	-542.4743	396.9697	59.31773	728.63636	164.33978
75.35354	-461.98936	407.0202	64.17343	738.68687	166.42461
85.40404	-399.0807	417.07071	68.86393	748.73737	168.47022
95.45455	-348.25449	427.12121	73.3975	758.78788	170.47786
105.50505	-306.12186	437.17172	77.78386	768.83838	172.44932
115.55556	-270.47072	447.22222	82.03025	778.88889	174.38507
125.60606	-239.79326	457.27273	86.1443	788.93939	176.2868
135.65657	-213.0231	467.32323	90.13301	798.9899	178.15517
145.70707	-189.38647	477.37374	94.00278	809.0404	179.99143
155.75758	-168.30311	487.42424	97.75998	819.09091	181.79647
165.80808	-149.33199	497.47475	101.409	829.14141	183.57142
175.85859	-132.13016	507.52525	104.9558	839.19192	185.3168
185.90909	-116.42495	517.57576	108.40493	849.24242	187.03364
195.9596	-102.00208	527.62626	111.76061	859.29293	188.72267
206.0101	-88.68557	537.67677	115.02806	869.34343	190.38486
216.06061	-76.33108	547.72727	118.20996	879.39394	192.02112
226.11111	-64.821	557.77778	121.31092	889.44444	193.63179
236.16162	-54.0567	567.82828	124.33397	899.49495	195.21747
246.21212	-43.9547	577.87879	127.28275	909.54545	196.7795
256.26263	-34.44554	587.92929	130.16025	919.59596	198.31789
266.31313	-25.46754	597.9798	132.96926	929.64646	199.83338
276.36364	-16.97146	608.0303	135.71279	939.69697	201.32673
286.41414	-8.91081	618.08081	138.39284	949.74747	202.79838
296.46465	-1.2486	628.13131	141.01248	959.79798	204.24901
306.51515	6.05042	638.18182	143.57417	969.84848	205.67902
316.56566	13.01474	648.23232	146.07987	979.89899	207.08881
326.61616	19.67084	658.28283	148.53141	989.94949	208.47923
336.66667	26.04201	668.33333	150.93123	1000	209.85038

Table S.18. Calculated free-energy function, ΔG ($\Delta G = G_T - G_{298}$), of studtite. Temperature and free-energy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	$G_T - G_{298}$	T	$G_T - G_{298}$	T	$G_T - G_{298}$
15.05051	-2445.14916	346.71717	-234.57102	678.38384	-298.65566
25.10101	-1467.35978	356.76768	-235.57386	688.43434	-300.92685
35.15152	-1050.00181	366.81818	-236.7085	698.48485	-303.19795
45.20202	-819.52619	376.86869	-237.96119	708.53535	-305.46862
55.25253	-674.15534	386.91919	-239.3215	718.58586	-307.7382
65.30303	-574.72446	396.9697	-240.77819	728.63636	-310.00609
75.35354	-502.94728	407.0202	-242.32237	738.68687	-312.27169
85.40404	-449.10892	417.07071	-243.94481	748.73737	-314.53479
95.45455	-407.57826	427.12121	-245.63886	758.78788	-316.79451
105.50505	-374.85179	437.17172	-247.39682	768.83838	-319.05069
115.55556	-348.63636	447.22222	-249.2133	778.88889	-321.30315
125.60606	-327.37098	457.27273	-251.08233	788.93939	-323.55111
135.65657	-309.95184	467.32323	-252.99847	798.9899	-325.79444
145.70707	-295.57809	477.37374	-254.95771	809.0404	-328.03302
155.75758	-283.65399	487.42424	-256.95543	819.09091	-330.26643
165.80808	-273.72683	497.47475	-258.98782	829.14141	-332.49429
175.85859	-265.44871	507.52525	-261.05188	839.19192	-334.71649
185.90909	-258.54312	517.57576	-263.1439	849.24242	-336.93296
195.9596	-252.79518	527.62626	-265.26092	859.29293	-339.14361
206.0101	-248.02726	537.67677	-267.40063	869.34343	-341.34783
216.06061	-244.09924	547.72727	-269.56046	879.39394	-343.54555
226.11111	-240.89061	557.77778	-271.73802	889.44444	-345.73699
236.16162	-238.30642	567.82828	-273.93154	899.49495	-347.92156
246.21212	-236.26534	577.87879	-276.13891	909.54545	-350.09923
256.26263	-234.6978	587.92929	-278.35862	919.59596	-352.27021
266.31313	-233.54566	597.9798	-280.58841	929.64646	-354.43421
276.36364	-232.76011	608.0303	-282.82781	939.69697	-356.59119
286.41414	-232.29751	618.08081	-285.07476	949.74747	-358.74088
296.46465	-232.12338	628.13131	-287.32816	959.79798	-360.88324
306.51515	-232.20305	638.18182	-289.58692	969.84848	-363.01825
316.56566	-232.51082	648.23232	-291.85007	979.89899	-365.14615
326.61616	-233.02196	658.28283	-294.1163	989.94949	-367.26641
336.66667	-233.71536	668.33333	-296.3851	1000	-369.37927

Table S.19. Calculated isobaric heat capacity function of soddyite. Temperature and heat capacity values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	C _p	T	C _p	T	C _p
15.05051	7.24976	346.71717	293.79305	678.38384	355.30402
25.10101	20.16971	356.76768	297.14511	688.43434	356.287
35.15152	35.13439	366.81818	300.34461	698.48485	357.24433
45.20202	50.54714	376.86869	303.3999	708.53535	358.17723
55.25253	65.84121	386.91919	306.31889	718.58586	359.08681
65.30303	80.7941	396.9697	309.10903	728.63636	359.97412
75.35354	95.22129	407.0202	311.77739	738.68687	360.84017
85.40404	108.9842	417.07071	314.33063	748.73737	361.68589
95.45455	122.01305	427.12121	316.77507	758.78788	362.51215
105.50505	134.2965	437.17172	319.11664	768.83838	363.31979
115.55556	145.86003	447.22222	321.36097	778.88889	364.10959
125.60606	156.74741	457.27273	323.51337	788.93939	364.88228
135.65657	167.00873	467.32323	325.57884	798.9899	365.63855
145.70707	176.69353	477.37374	327.56211	809.0404	366.37905
155.75758	185.84759	487.42424	329.46763	819.09091	367.10438
165.80808	194.51171	497.47475	331.29963	829.14141	367.81513
175.85859	202.72161	507.52525	333.06206	839.19192	368.51185
185.90909	210.50845	517.57576	334.75868	849.24242	369.19503
195.9596	217.89949	527.62626	336.39301	859.29293	369.86517
206.0101	224.91883	537.67677	337.9684	869.34343	370.52272
216.06061	231.58806	547.72727	339.48798	879.39394	371.16812
226.11111	237.92674	557.77778	340.9547	889.44444	371.80176
236.16162	243.95288	567.82828	342.37137	899.49495	372.42403
246.21212	249.68322	577.87879	343.7406	909.54545	373.0353
256.26263	255.13345	587.92929	345.06489	919.59596	373.63591
266.31313	260.31838	597.9798	346.34656	929.64646	374.22619
276.36364	265.25204	608.0303	347.5878	939.69697	374.80643
286.41414	269.94775	618.08081	348.79069	949.74747	375.37695
296.46465	274.41818	628.13131	349.95718	959.79798	375.938
306.51515	278.6754	638.18182	351.08909	969.84848	376.48987
316.56566	282.73088	648.23232	352.18815	979.89899	377.03279
326.61616	286.5955	658.28283	353.25599	989.94949	377.567
336.66667	290.27961	668.33333	354.29414	1000	378.09274

Table S.20. Calculated entropy function of soddyite. Temperature and entropy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	S	T	S	T	S
15.05051	2.46013	346.71717	358.89784	678.38384	578.71705
25.10101	9.05715	356.76768	367.34107	688.43434	583.94959
35.15152	18.20173	366.81818	375.64088	698.48485	589.12047
45.20202	28.89361	376.86869	383.80075	708.53535	594.23078
55.25253	40.52853	386.91919	391.82441	718.58586	599.28223
65.30303	52.75419	396.9697	399.71552	728.63636	604.27593
75.35354	65.33421	407.0202	407.47768	738.68687	609.21341
85.40404	78.10818	417.07071	415.11414	748.73737	614.09551
95.45455	90.95166	427.12121	422.62813	758.78788	618.92376
105.50505	103.77621	437.17172	430.02312	768.83838	623.69921
115.55556	116.51995	447.22222	437.30202	778.88889	628.42294
125.60606	129.137	457.27273	444.46799	788.93939	633.09619
135.65657	141.59594	467.32323	451.5242	798.9899	637.71994
145.70707	153.87819	477.37374	458.47302	809.0404	642.2953
155.75758	165.96837	487.42424	465.31789	819.09091	646.82317
165.80808	177.85997	497.47475	472.06098	829.14141	651.30469
175.85859	189.54793	507.52525	478.70526	839.19192	655.74051
185.90909	201.03155	517.57576	485.25297	849.24242	660.13185
195.9596	212.30903	527.62626	491.7069	859.29293	664.4794
206.0101	223.38362	537.67677	498.06939	869.34343	668.78415
216.06061	234.25626	547.72727	504.34261	879.39394	673.04687
226.11111	244.92991	557.77778	510.52901	889.44444	677.26858
236.16162	255.40849	567.82828	516.63065	899.49495	681.4497
246.21212	265.69535	577.87879	522.64965	909.54545	685.59134
256.26263	275.79419	587.92929	528.58801	919.59596	689.69412
266.31313	285.70912	597.9798	534.44775	929.64646	693.75865
276.36364	295.44446	608.0303	540.23102	939.69697	697.78591
286.41414	305.00357	618.08081	545.93937	949.74747	701.77645
296.46465	314.39092	628.13131	551.57488	959.79798	705.73078
306.51515	323.61123	638.18182	557.13909	969.84848	709.64992
316.56566	332.66781	648.23232	562.63384	979.89899	713.53419
326.61616	341.5651	658.28283	568.06065	989.94949	717.38432
336.66667	350.30694	668.33333	573.42116	1000	721.20082

Table S.21. Calculated enthalpy function, ΔH ($\Delta H = H_T - H_{298}$), of soddyite. Temperature and enthalpy values are given in K and $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ units, respectively.

T	$H_T - H_{298}$	T	$H_T - H_{298}$	T	$H_T - H_{298}$
15.05051	-3203.36362	346.71717	39.89811	678.38384	182.16309
25.10101	-1915.3483	356.76768	47.09837	688.43434	184.69806
35.15152	-1359.82804	366.81818	53.99351	698.48485	187.17388
45.20202	-1047.95	376.86869	60.6044	708.53535	189.59292
55.25253	-846.73759	386.91919	66.94947	718.58586	191.95721
65.30303	-705.13	396.9697	73.04525	728.63636	194.26869
75.35354	-599.33632	407.0202	78.90755	738.68687	196.52919
85.40404	-516.78339	417.07071	84.55035	748.73737	198.74044
95.45455	-450.20323	427.12121	89.98604	758.78788	200.90424
105.50505	-395.10208	437.17172	95.22698	768.83838	203.02213
115.55556	-348.54939	447.22222	100.28413	778.88889	205.09574
125.60606	-308.54887	457.27273	105.16698	788.93939	207.12631
135.65657	-273.69218	467.32323	109.88523	798.9899	209.1156
145.70707	-242.95631	477.37374	114.44725	809.0404	211.06456
155.75758	-215.57991	487.42424	118.86146	819.09091	212.97481
165.80808	-190.98267	497.47475	123.1349	829.14141	214.84749
175.85859	-168.71411	507.52525	127.27472	839.19192	216.68364
185.90909	-148.42189	517.57576	131.28756	849.24242	218.48458
195.9596	-129.8216	527.62626	135.17883	859.29293	220.25124
206.0101	-112.68493	537.67677	138.95491	869.34343	221.98468
216.06061	-96.82382	547.72727	142.62082	879.39394	223.68605
226.11111	-82.08417	557.77778	146.18143	889.44444	225.35615
236.16162	-68.33609	567.82828	149.64148	899.49495	226.9959
246.21212	-55.47039	577.87879	153.00539	909.54545	228.60631
256.26263	-43.39455	587.92929	156.27726	919.59596	230.18808
266.31313	-32.02955	597.9798	159.46113	929.64646	231.74213
276.36364	-21.30745	608.0303	162.56058	939.69697	233.26922
286.41414	-11.16856	618.08081	165.57913	949.74747	234.76997
296.46465	-1.56212	628.13131	168.52009	959.79798	236.24532
306.51515	7.55756	638.18182	171.38637	969.84848	237.69581
316.56566	16.23	648.23232	174.18107	979.89899	239.1222
326.61616	24.49056	658.28283	176.90711	989.94949	240.525
336.66667	32.37076	668.33333	179.56686	1000	241.90502

Table S.22. Calculated free-energy function, ΔG ($\Delta G = G_T - G_{298}$), of soddyite. Temperature and free-energy values are given in K and $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ units, respectively.

T	$G_T - G_{298}$	T	$G_T - G_{298}$	T	$G_T - G_{298}$
15.05051	-3205.82479	346.71717	-318.99939	678.38384	-396.55396
25.10101	-1924.40544	356.76768	-320.24269	688.43434	-399.25153
35.15152	-1378.02977	366.81818	-321.64705	698.48485	-401.94641
45.20202	-1076.84361	376.86869	-323.19634	708.53535	-404.63787
55.25253	-887.2683	386.91919	-324.87494	718.58586	-407.32502
65.30303	-757.88419	396.9697	-326.67027	728.63636	-410.00724
75.35354	-664.67213	407.0202	-328.56984	738.68687	-412.68406
85.40404	-594.89016	417.07071	-330.56379	748.73737	-415.35507
95.45455	-541.15363	427.12121	-332.64181	758.78788	-418.01952
105.50505	-498.87829	437.17172	-334.79587	768.83838	-420.67707
115.55556	-465.06934	447.22222	-337.01789	778.88889	-423.32735
125.60606	-437.68588	457.27273	-339.30101	788.93939	-425.96988
135.65657	-415.28812	467.32323	-341.63897	798.9899	-428.60449
145.70707	-396.8345	477.37374	-344.02577	809.0404	-431.23075
155.75758	-381.54829	487.42424	-346.45643	819.09091	-433.84835
165.80808	-368.84264	497.47475	-348.92608	829.14141	-436.4572
175.85859	-358.26273	507.52525	-351.43054	839.19192	-439.05687
185.90909	-349.4528	517.57576	-353.96564	849.24242	-441.64727
195.9596	-342.13063	527.62626	-356.52807	859.29293	-444.22816
206.0101	-336.06796	537.67677	-359.11448	869.34343	-446.79947
216.06061	-331.08008	547.72727	-361.72201	879.39394	-449.36096
226.11111	-327.01408	557.77778	-364.34758	889.44444	-451.91242
236.16162	-323.74458	567.82828	-366.98917	899.49495	-454.4538
246.21212	-321.16574	577.87879	-369.64426	909.54545	-456.98503
256.26263	-319.18874	587.92929	-372.31075	919.59596	-459.50591
266.31313	-317.73867	597.9798	-374.98662	929.64646	-462.01653
276.36364	-316.75148	608.0303	-377.67044	939.69697	-464.51669
286.41414	-316.17213	618.08081	-380.36024	949.74747	-467.00635
296.46465	-315.95304	628.13131	-383.05479	959.79798	-469.48546
306.51515	-316.05327	638.18182	-385.75272	969.84848	-471.95411
316.56566	-316.43743	648.23232	-388.45258	979.89899	-474.41199
326.61616	-317.07417	658.28283	-391.15354	989.94949	-476.8592
336.66667	-317.93619	668.33333	-393.8543	1000	-479.2958

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