Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Becquerelite mineral phase: crystal structure and thermodynamic and mechanic stability by using periodic DFT

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

T	C_P	T	C_P	T	C_P
10	1.59646	350	158.73070	690	193.50098
20	6.74505	360	160.46961	700	194.10347
30	13.95060	370	162.13674	710	194.69408
40	22.20754	380	163.73601	720	195.27332
50	30.92287	390	165.27110	730	195.84167
60	39.65372	400	166.74548	740	196.39958
70	48.11604	410	168.16244	750	196.94747
80	56.15642	420	169.52506	760	197.48575
90	63.70929	430	170.83629	770	198.01478
100	70.76223	440	172.09887	780	198.53490
110	77.33249	450	173.31543	790	199.04646
120	83.45203	460	174.48844	800	199.54974
130	89.15862	470	175.62023	810	200.04503
140	94.49062	480	176.71301	820	200.53261
150	99.48419	490	177.76886	830	201.01272
160	104.17209	500	178.78977	840	201.48559
170	108.58321	510	179.77759	850	201.95146
180	112.74272	520	180.73409	860	202.41051
190	116.67242	530	181.66093	870	202.86296
200	120.39118	540	182.55967	880	203.30897
210	123.91541	550	183.43181	890	203.74873
220	127.25944	560	184.27873	900	204.18238
230	130.43596	570	185.10177	910	204.61010
240	133.45622	580	185.90215	920	205.03201
250	136.33036	590	186.68104	930	205.44825
260	139.06756	600	187.43955	940	205.85896
270	141.67618	610	188.17872	950	206.26425
280	144.16391	620	188.89952	960	206.66424
290	146.53785	630	189.60286	970	207.05903
300	148.80458	640	190.28960	980	207.44873
310	150.97022	650	190.96055	990	207.83344
320	153.04047	660	191.61648	1000	208.21325
330	155.02068	670	192.25809	-	-
340	156.91586	680	192.88604	-	-

Table S.2. Calculated entropy function, S, of becquerelite. Temperature and entropy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	S	T	S	T	S
10	0.67942	350	196.97227	690	317.31869
20	3.20211	360	201.46840	700	320.10725
30	7.25114	370	205.88796	710	322.86477
40	12.37826	380	210.23328	720	325.59187
50	18.26548	390	214.50637	730	328.28924
60	24.67746	400	218.70933	740	330.95761
70	31.43067	410	222.84424	750	333.59755
80	38.38558	420	226.91301	760	336.20974
90	45.44057	430	230.91754	770	338.79471
100	52.52259	440	234.85955	780	341.35314
110	59.57859	450	238.74080	790	343.88557
120	66.57320	460	242.56298	800	346.39249
130	73.48069	470	246.32773	810	348.87447
140	80.28556	480	250.03671	820	351.33206
150	86.97670	490	253.69127	830	353.76569
160	93.54856	500	257.29301	840	356.17588
170	99.99759	510	260.84336	850	358.56309
180	106.32304	520	264.34359	860	360.92782
190	112.52496	530	267.79511	870	363.27046
200	118.60479	540	271.19912	880	365.59150
210	124.56486	550	274.55697	890	367.89129
220	130.40723	560	277.86978	900	370.17026
230	136.13468	570	281.13871	910	372.42878
240	141.75035	580	284.36493	920	374.66731
250	147.25704	590	287.54952	930	376.88614
260	152.65788	600	290.69348	940	379.08564
270	157.95557	610	293.79783	950	381.26622
280	163.15339	620	296.86357	960	383.42818
290	168.25392	630	299.89166	970	385.57183
300	173.26031	640	302.88303	980	387.69754
310	178.17520	650	305.83852	990	389.80556
320	183.00126	660	308.75896	1000	391.89627
330	187.74108	670	311.64534	-	-
340	192.39731	680	314.49831	-	-

Table S.3. Calculated enthalpy function, $^{\Delta H}$ $(\Delta H = H_T - H_{298})$, of becquerelite. Temperature and enthalpy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	$H_T - H_{298}$	T	$H_T - H_{298}$	T	$H_T - H_{298}$
10	-2629.36792	350	22.77841	690	99.87522
20	-1312.71807	360	26.57909	700	101.21705
30	-871.73489	370	30.22050	710	102.52951
40	-649.29751	380	33.71311	720	103.81361
50	-514.12810	390	37.06691	730	105.07035
60	-422.55649	400	40.29052	740	106.30078
70	-355.91743	410	43.39217	750	107.50575
80	-304.90595	420	46.37925	760	108.68620
90	-264.36377	430	49.25843	770	109.84288
100	-231.19955	440	52.03597	780	110.97661
110	-203.44644	450	54.71768	790	112.08819
120	-179.79019	460	57.30875	800	113.17832
130	-159.31877	470	59.81402	810	114.24774
140	-141.37785	480	62.23811	820	115.29700
150	-125.48493	490	64.58516	830	116.32685
160	-111.27635	500	66.85907	840	117.33782
170	-98.47191	510	69.06351	850	118.33053
180	-86.85232	520	71.20188	860	119.30558
190	-76.24298	530	73.27731	870	120.26340
200	-66.50322	540	75.29284	880	121.20456
210	-57.51894	550	77.25109	890	122.12958
220	-49.19518	560	79.15476	900	123.03887
230	-41.45364	570	81.00631	910	123.93291
240	-34.22809	580	82.80795	920	124.81214
250	-27.46286	590	84.56200	930	125.67696
260	-21.10995	600	86.27031	940	126.52779
270	-15.12876	610	87.93488	950	127.36497
280	-9.48392	620	89.55755	960	128.18891
290	-4.14450	630	91.14000	970	129.00000
300	0.91641	640	92.68393	980	129.79851
310	5.72214	650	94.19068	990	130.58479
320	10.29372	660	95.66189	1000	131.35917
330	14.64963	670	97.09883	-	-
340	18.80630	680	98.50292	-	-

Table S.4. Calculated free-energy function, $^{\Delta G}$ ($\Delta G = G_T - H_{298}$), of becquerelite. Temperature and free-energy values are given in K and $J \cdot K^{-1} \cdot mol^{-1}$ units, respectively.

T	$G_T - H_{298}$	T	$G_T - H_{298}$	T	$G_T - H_{298}$
10	-2630.04781	350	-174.19387	690	-217.44347
20	-1315.92018	360	-174.88921	700	-218.89021
30	-878.98603	370	-175.66746	710	-220.33526
40	-661.67477	380	-176.52007	720	-221.77826
50	-532.39358	390	-177.43946	730	-223.21884
60	-447.23395	400	-178.41881	740	-224.65677
70	-387.34810	410	-179.45207	750	-226.09174
80	-343.29153	420	-180.53377	760	-227.52354
90	-309.80434	430	-181.65911	770	-228.95188
100	-283.72214	440	-182.82348	780	-230.37653
110	-263.02504	450	-184.02312	790	-231.79733
120	-246.36339	460	-185.25424	800	-233.21416
130	-232.79946	470	-186.51371	810	-234.62674
140	-221.66341	480	-187.79860	820	-236.03501
150	-212.46190	490	-189.10612	830	-237.43884
160	-204.82491	500	-190.43394	840	-238.83807
170	-198.46949	510	-191.77977	850	-240.23256
180	-193.17513	520	-193.14171	860	-241.62224
190	-188.76773	530	-194.51772	870	-243.00706
200	-185.10821	540	-195.90635	880	-244.38690
210	-182.08380	550	-197.30588	890	-245.76171
220	-179.60241	560	-198.71502	900	-247.13138
230	-177.58850	570	-200.13240	910	-248.49587
240	-175.97860	580	-201.55699	920	-249.85516
250	-174.71990	590	-202.98752	930	-251.20917
260	-173.76784	600	-204.42317	940	-252.55790
270	-173.08448	610	-205.86289	950	-253.90125
280	-172.63716	620	-207.30603	960	-255.23923
290	-172.39842	630	-208.75166	970	-256.57184
300	-172.34390	640	-210.19910	980	-257.89903
310	-172.45307	650	-211.64778	990	-259.22077
320	-172.70755	660	-213.09708	1000	-260.53710
330	-173.09145	670	-214.54644	-	-
340	-173.59100	680	-215.99539	-	-