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# SUPPORTING INFORMATION

## Thermodynamic and Mechanical Properties of Rutherfordine Mineral Based on Density Functional Theory

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**APPENDIX A.** Calculated thermodynamic functions.

**Table A.1.** Calculated isobaric heat capacity function. Temperature and heat capacity values are given in units K and J/(K·mol), respectively.

T	C <sub>p</sub>	T	C <sub>p</sub>	T	C <sub>p</sub>	T	C <sub>p</sub>
5	0.4293	256.26263	107.42752	507.52525	140.9014	758.78788	155.86372
15.05051	4.69165	266.31313	109.34672	517.57576	141.75582	768.83838	156.25559
25.10101	9.92651	276.36364	111.20344	527.62626	142.58284	778.88889	156.6362
35.15152	16.19379	286.41414	113.00071	537.67677	143.38339	788.93939	157.00595
45.20202	23.1633	296.46465	114.74107	547.72727	144.15838	798.9899	157.36521
55.25253	30.50212	306.51515	116.4267	557.77778	144.90867	809.0404	157.71434
65.30303	37.87873	316.56566	118.05953	567.82828	145.63512	819.09091	158.05368
75.35354	44.98538	326.61616	119.64127	577.87879	146.33856	829.14141	158.38357
85.40404	51.60986	336.66667	121.1735	587.92929	147.0198	839.19192	158.70433
95.45455	57.65034	346.71717	122.6577	597.9798	147.6796	849.24242	159.01626
105.50505	63.09102	356.76768	124.09527	608.0303	148.31871	859.29293	159.31968
115.55556	67.96931	366.81818	125.48755	618.08081	148.93788	869.34343	159.61485
125.60606	72.34877	376.86869	126.83582	628.13131	149.53779	879.39394	159.90206
135.65657	76.30095	386.91919	128.14135	638.18182	150.11913	889.44444	160.18157
145.70707	79.89487	396.9697	129.40538	648.23232	150.68256	899.49495	160.45363
155.75758	83.19186	407.0202	130.6291	658.28283	151.2287	909.54545	160.7185
165.80808	86.24375	417.07071	131.81372	668.33333	151.75817	919.59596	160.9764
175.85859	89.09284	427.12121	132.96039	678.38384	152.27156	929.64646	161.22756
185.90909	91.77295	437.17172	134.07026	688.43434	152.76944	939.69697	161.47221
195.9596	94.31063	447.22222	135.14447	698.48485	153.25235	949.74747	161.71055
206.0101	96.72654	457.27273	136.18413	708.53535	153.72082	959.79798	161.94278
216.06061	99.03665	467.32323	137.19031	718.58586	154.17535	969.84848	162.1691
226.11111	101.2533	477.37374	138.16409	728.63636	154.61645	979.89899	162.3897
236.16162	103.386	487.42424	139.10652	738.68687	155.04458	989.94949	162.60476
246.21212	105.44214	497.47475	140.01863	748.73737	155.46019	1000	162.81445

**Table A.2.** Calculated entropy function. Temperature and entropy values are given in units K and J/(K·mol), respectively.

T	S	T	S	T	S	T	S
5	0.1399	256.26263	126.39578	507.52525	211.30287	758.78788	271.12378
15.05051	2.34354	266.31313	130.2552	517.57576	214.19743	768.83838	273.05348
25.10101	5.92618	276.36364	134.59704	527.62626	217.09199	778.88889	275.46562
35.15152	10.23994	286.41414	138.45645	537.67677	219.50413	788.93939	277.39532
45.20202	15.14086	296.46465	142.31586	547.72727	222.39869	798.9899	279.32503
55.25253	20.5	306.51515	146.17527	557.77778	224.81082	809.0404	281.25474
65.30303	26.19866	316.56566	150.03469	567.82828	227.22295	819.09091	283.18444
75.35354	32.12238	326.61616	153.8941	577.87879	230.11751	829.14141	285.11415
85.40404	38.16646	336.66667	157.27109	587.92929	232.52964	839.19192	287.04386
95.45455	44.24378	346.71717	161.1305	597.9798	234.94178	849.24242	288.97356
105.50505	50.17237	356.76768	164.50749	608.0303	237.35391	859.29293	290.90327
115.55556	56.44392	366.81818	167.88447	618.08081	239.76604	869.34343	292.83298
125.60606	62.23304	376.86869	171.26146	628.13131	242.17818	879.39394	294.28026
135.65657	68.02216	386.91919	174.63845	638.18182	244.59031	889.44444	296.20996
145.70707	73.32885	396.9697	178.01543	648.23232	247.00244	899.49495	298.13967
155.75758	78.63554	407.0202	181.39242	658.28283	249.41458	909.54545	300.06938
165.80808	83.94224	417.07071	184.76941	668.33333	251.82671	919.59596	301.51666
175.85859	89.24893	427.12121	187.66397	678.38384	253.75642	929.64646	303.44636
185.90909	94.55562	437.17172	191.04095	688.43434	256.16855	939.69697	305.37607
195.9596	99.37989	447.22222	193.93551	698.48485	258.58068	949.74747	306.82335
206.0101	104.20416	457.27273	196.83007	708.53535	260.51039	959.79798	308.75306
216.06061	108.546	467.32323	199.72463	718.58586	262.92252	969.84848	310.20034
226.11111	113.37026	477.37374	202.61919	728.63636	264.85223	979.89899	312.13004
236.16162	117.7121	487.42424	205.51375	738.68687	267.26436	989.94949	313.57732
246.21212	122.05394	497.47475	208.40831	748.73737	269.19407	1000	315.0246

**Table A.3.** Calculated enthalpy function,  $H_T-H_{298}$ . Temperature and enthalpy values are given in units K and J/(K·mol), respectively.

T	$H_T-H_{298}$	T	$H_T-H_{298}$	T	$H_T-H_{298}$	T	$H_T-H_{298}$
5	-4230.55345	256.26263	-18.19806	507.52525	53.38394	758.78788	85.16243
15.05051	-1403.85635	266.31313	-13.4209	517.57576	55.09138	768.83838	86.08908
25.10101	-838.86425	276.36364	-8.92139	527.62626	56.75023	778.88889	86.99677
35.15152	-595.29722	286.41414	-4.67533	537.67677	58.36231	788.93939	87.88623
45.20202	-458.56999	296.46465	-0.65533	547.72727	59.92933	798.9899	88.75814
55.25253	-370.27469	306.51515	3.15613	557.77778	61.45458	809.0404	89.61256
65.30303	-308.02744	316.56566	6.77891	567.82828	62.93772	819.09091	90.45013
75.35354	-261.41186	326.61616	10.22747	577.87879	64.38264	829.14141	91.27205
85.40404	-224.96014	336.66667	13.51599	587.92929	65.78882	839.19192	92.07774
95.45455	-195.51736	346.71717	16.65838	597.9798	67.15984	849.24242	92.86776
105.50505	-171.13537	356.76768	19.66565	608.0303	68.49663	859.29293	93.64324
115.55556	-150.54794	366.81818	22.54625	618.08081	69.79932	869.34343	94.40411
125.60606	-132.88261	376.86869	25.30906	628.13131	71.07031	879.39394	95.15143
135.65657	-117.52901	386.91919	27.96325	638.18182	72.31109	889.44444	95.88457
145.70707	-104.03527	396.9697	30.51585	648.23232	73.52158	899.49495	96.60455
155.75758	-92.05683	407.0202	32.97321	658.28283	74.7039	909.54545	97.31127
165.80808	-81.34143	417.07071	35.3399	668.33333	75.85861	919.59596	98.00569
175.85859	-71.68073	427.12121	37.62457	678.38384	76.98692	929.64646	98.68821
185.90909	-62.91667	437.17172	39.82847	688.43434	78.08929	939.69697	99.35818
195.9596	-54.91619	447.22222	41.9592	698.48485	79.16754	949.74747	100.01702
206.0101	-47.57692	457.27273	44.01842	708.53535	80.222	959.79798	100.66407
216.06061	-40.81104	467.32323	46.01178	718.58586	81.25302	969.84848	101.3002
226.11111	-34.54423	477.37374	47.94142	728.63636	82.26221	979.89899	101.92574
236.16162	-28.72093	487.42424	49.81127	738.68687	83.24916	989.94949	102.54052
246.21212	-23.28489	497.47475	51.62497	748.73737	84.21606	1000	103.14537

**Table A.4.** Calculated free energy function,  $G_T-H_{298}$ . Temperature and free energy values are given in units K and J/(K·mol), respectively.

T	$G_T-H_{298}$	T	$G_T-H_{298}$	T	$G_T-H_{298}$	T	$G_T-H_{298}$
5	-4230.69326	256.26263	-144.47936	507.52525	-157.9626	758.78788	-186.04858
15.05051	-1406.19989	266.31313	-143.87075	517.57576	-159.02623	768.83838	-187.17491
25.10101	-844.78382	276.36364	-143.45653	527.62626	-160.10146	778.88889	-188.29941
35.15152	-605.53548	286.41414	-143.21455	537.67677	-161.18763	788.93939	-189.42034
45.20202	-473.71452	296.46465	-143.12241	547.72727	-162.28327	798.9899	-190.53842
55.25253	-390.77579	306.51515	-143.16538	557.77778	-163.38613	809.0404	-191.65318
65.30303	-334.22355	316.56566	-143.326	567.82828	-164.49753	819.09091	-192.76473
75.35354	-293.53158	326.61616	-143.59196	577.87879	-165.61451	829.14141	-193.87318
85.40404	-263.12314	336.66667	-143.95093	587.92929	-166.73679	839.19192	-194.9775
95.45455	-239.76001	346.71717	-144.39484	597.9798	-167.86329	849.24242	-196.07841
105.50505	-221.42423	356.76768	-144.91381	608.0303	-168.99382	859.29293	-197.17546
115.55556	-206.79981	366.81818	-145.50034	618.08081	-170.12738	869.34343	-198.26879
125.60606	-194.9882	376.86869	-146.14776	628.13131	-171.26384	879.39394	-199.35852
135.65657	-185.35352	386.91919	-146.84882	638.18182	-172.40155	889.44444	-200.44369
145.70707	-177.44201	396.9697	-147.59824	648.23232	-173.54118	899.49495	-201.52553
155.75758	-170.90458	407.0202	-148.39243	658.28283	-174.6812	909.54545	-202.60255
165.80808	-165.48557	417.07071	-149.22584	668.33333	-175.82157	919.59596	-203.67597
175.85859	-160.98497	427.12121	-150.09457	678.38384	-176.96229	929.64646	-204.74486
185.90909	-157.24606	437.17172	-150.99509	688.43434	-178.10264	939.69697	-205.80988
195.9596	-154.14424	447.22222	-151.92418	698.48485	-179.24263	949.74747	-206.87014
206.0101	-151.58394	457.27273	-152.87994	708.53535	-180.38092	959.79798	-207.92628
216.06061	-149.47842	467.32323	-153.8586	718.58586	-181.51826	969.84848	-208.97845
226.11111	-147.76704	477.37374	-154.8587	728.63636	-182.65401	979.89899	-210.02626
236.16162	-146.39129	487.42424	-155.87695	738.68687	-183.78759	989.94949	-211.06937
246.21212	-145.30814	497.47475	-156.91223	748.73737	-184.91909	1000	-212.10839

**Table A.5.** Calculated Debye temperature function,  $\theta_{\text{Debye}}$ . All values are given in K units.

T	$\theta_{\text{Debye}}$	T	$\theta_{\text{Debye}}$	T	$\theta_{\text{Debye}}$	T	$\theta_{\text{Debye}}$
5	158.23	256.26263	842.37149	507.52525	1075.73832	758.78788	1157.37723
15.05051	214.53138	266.31313	857.59832	517.57576	1080.75916	768.83838	1159.3997
25.10101	277.57936	276.36364	872.15777	527.62626	1085.5786	778.88889	1161.30081
35.15152	326.97289	286.41414	886.07979	537.67677	1090.17826	788.93939	1163.10002
45.20202	367.46264	296.46465	899.38664	547.72727	1094.64686	798.9899	1164.94219
55.25253	401.73049	306.51515	912.0999	557.77778	1098.87066	809.0404	1166.67223
65.30303	431.72708	316.56566	924.24511	567.82828	1102.98162	819.09091	1168.28909
75.35354	459.04221	326.61616	935.84721	577.87879	1106.89878	829.14141	1169.953
85.40404	484.79819	336.66667	946.93037	587.92929	1110.68758	839.19192	1171.57989
95.45455	509.67735	346.71717	957.518	597.9798	1114.31904	849.24242	1173.0142
105.50505	534.07047	356.76768	967.63275	608.0303	1117.82105	859.29293	1174.49868
115.55556	558.14883	366.81818	977.29654	618.08081	1121.18344	869.34343	1176.03374
125.60606	581.95215	376.86869	986.53066	628.13131	1124.435	879.39394	1177.35057
135.65657	605.45267	386.91919	995.35589	638.18182	1127.54118	889.44444	1178.65186
145.70707	628.5858	396.9697	1003.7926	648.23232	1130.58062	899.49495	1180.00585
155.75758	651.27175	407.0202	1011.86095	658.28283	1133.44014	909.54545	1181.38281
165.80808	673.42886	417.07071	1019.58104	668.33333	1136.30635	919.59596	1182.49491
175.85859	694.98988	427.12121	1026.96269	678.38384	1138.92838	929.64646	1183.66134
185.90909	715.90842	437.17172	1034.01602	688.43434	1141.56286	939.69697	1184.88199
195.9596	736.14451	447.22222	1040.77113	698.48485	1144.05563	949.74747	1186.12396
206.0101	755.66778	457.27273	1047.24789	708.53535	1146.46135	959.79798	1187.09458
216.06061	774.45852	467.32323	1053.45179	718.58586	1148.87479	969.84848	1188.12049
226.11111	792.51401	477.37374	1059.37269	728.63636	1151.05262	979.89899	1189.20139
236.16162	809.84994	487.42424	1065.06239	738.68687	1153.26132	989.94949	1190.33694
246.21212	826.4595	497.47475	1070.53419	748.73737	1155.39245	1000	1191.23935

## APPENDIX B. Temperature dependent Debye temperature.

Debye temperature,  $\Theta_D$ , is an important quantity which gives a relative idea for a temperature scale above which the vibrations within a solid behave classically and the heat capacity follows the Dulong-Petit law<sup>1</sup>. Below the Debye temperature the quantum effects are important. Debye temperature may be estimated in terms of the mean sound velocity of a crystal or elasticity constants<sup>2</sup>. Thus, its temperature dependence comes from that of elasticity constants and it is very slight.

A popular representation of the experimental data on heat capacity is based on the comparison of the actual heat capacity to that predicted by the Debye model. This leads to the concept of the temperature dependent Debye temperature,  $\Theta_D(T)$ . The constant volume heat capacity in the Debye model is given by<sup>1</sup>

$$C_v^D = 9 nk \left( \frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

Where  $n$  is the number of atoms per cell and  $k$  is the Boltzmann constant. Once the actual heat capacity value at a given  $T$  is known, one may determine  $\Theta_D$  at that temperature by inverting this equation.

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