

$T_a = 273 \text{ K}$
 $T = 25 \text{ }^\circ\text{C}$
 $T^\circ = 298 \text{ K}$

Výpočet s lineární závislostí H
 (c_p konstantní)

$H_{25} = 100 \text{ J/mol}$
 $c_p = 8 \text{ J/mol K}$
 $T = 373$
 $H_{373} = ? \text{ J/mol}$

$$c_p = \frac{q}{\Delta T} = \frac{\Delta H}{\Delta T}$$

$$\Delta H = c_p \Delta T$$

$$H_{373} - H_{298} = c_p (373 - 298)$$

$$H_{373} = H_{298} + c_p (373 - 298)$$

$H_{373} = 700 \text{ J/mol}$

Graf c_p konstantní
 T H
 (K) (J/mol)
 298 100
 373 700

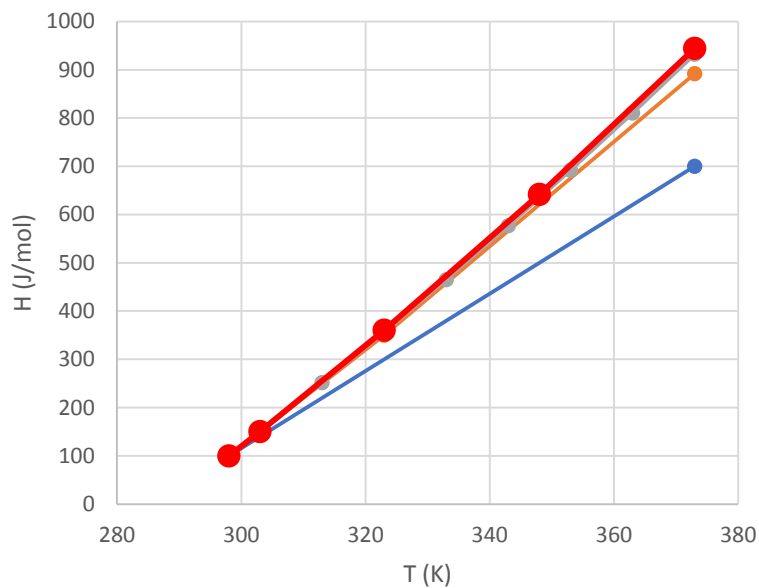
Výpočet s nelineární závislostí H
 (c_p funkcí teploty, krok 25)

$$c_p = k \times T$$

$$k = 0.033557 \quad 0.026846$$

$$H_{i+1} = H_i + \Delta H_i$$

T ($^\circ\text{C}$)	T (K)	H (J/mol)
25	298	100.0
50	323	350.0
100	373	891.9



—●— (c_p konstantní) —●— (c_p funkcí teploty, krok 25)
 —●— (c_p funkcí teploty, krok 10) —●— (H z integrace)

Výpočet s nelineární závislostí H

(c_p funkcí teploty, krok 10)

10
0.033557

c_p (J/mol K)	ΔH_i (J/mol)	T (°C)	T (K)	H (J/mol)	c_p (J/mol K)	ΔH_i (J/mol)
10.00	250.0		25	298	10.00	50.0
10.84	541.9		30	303	10.17	101.7
12.52			40	313	10.50	105.0
			50	323	10.84	108.4
			60	333	11.17	111.7
			70	343	11.51	115.1
			80	353	11.85	118.5
			90	363	12.18	121.8
			100	373	12.52	

Výpočet s nelineární závislostí H

(H z integrace)

$$dH = c_p dT = kT dT$$

$$\int_{H_{T^0}}^{H_T} dH = \int_{T^0}^T kT dT$$

$$[H]_{T^0}^T = k \left[\frac{1}{2} T^2 \right]_{T^0}^T$$

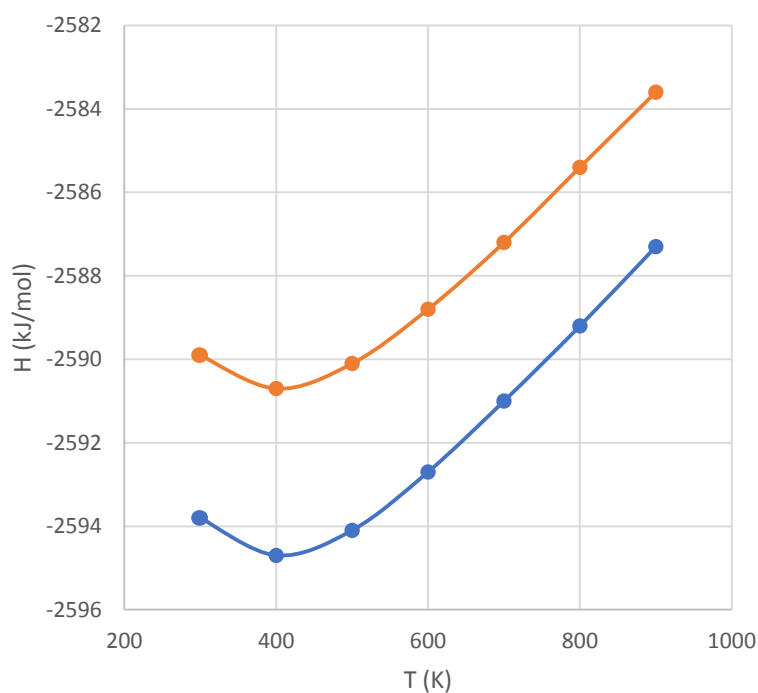
$$H_T - H_{T^0} = \frac{1}{2} k (T^2 - T^{0^2})$$

$$H_T = H_{T^0} + \frac{1}{2} k (T^2 - T^{0^2})$$

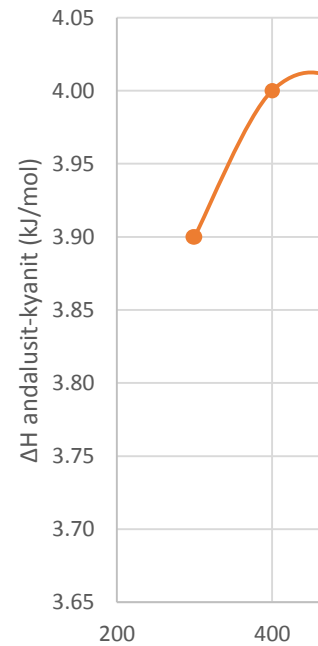
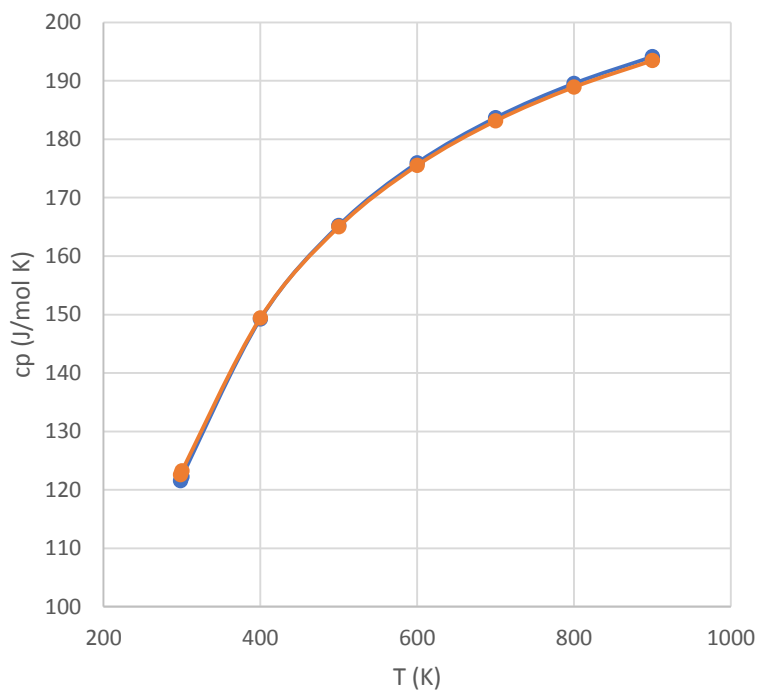
T (°C)	T (K)	H (J/mol)
25	298	100.0
30	303	150.4
50	323	360.5
75	348	641.9
100	373	944.4

T = 273.15 kyanit

T (°C)	kyanit			H (kJ/mol)				
	T (K)	cp (J/mol K)	S	(HT-H298)/ -(GT-H298)	H _{kyanit}	AfGO		
25	298.15	121.58	82.8	0.00	82.8	-2593.8	-2443.1	
26.85	300	122.26	83.55	0.75	82.8	-2593.8	-2442.2	
126.85	400	149.25	122.81	34.84	87.97	-2594.7	-2391.4	
226.85	500	165.25	157.97	59.44	98.53	-2594.1	-2340.6	
326.85	600	175.97	189.1	78.02	111.08	-2592.7	-2290.1	
426.85	700	183.7	216.84	92.59	124.24	-2591.0	-2239.8	
526.85	800	189.56	241.77	104.36	137.4	-2589.2	-2189.7	
626.85	900	194.15	264.37	114.09	150.27	-2587.3	-2139.9	
726.85	1000	197.84	285.02	122.29	162.73	-2606.8	-2088.8	
826.85	1100	200.85	304.02	129.3	174.72	-2604.6	-2037.1	
926.85	1200	203.35	321.61	135.37	186.24	-2602.3	-1985.6	
1026.85	1300	205.44	337.97	140.68	197.29	-2599.9	-1934.2	
1126.85	1400	207.2	353.26	145.37	207.89	-2597.5	-1883.2	
1226.85	1500	208.7	367.61	149.54	218.06	-2595.0	-1832.2	
1326.85	1600	209.97	381.12	153.28	227.84	-2592.5	-1781.5	
1426.85	1700	211.06	393.88	156.65	237.23	-2640.1	-1730.4	
1526.85	1800	211.99	405.97	159.7	246.27	-2637.3	-1677	



LogKf	andalusit		ST	(HT-H298)/-(GT-H298)	$H_{\text{andalusit}}$	AfGO	
	Temp.	cp					
428.01	298.15	122.6	91.39	0.00	91.39	-2589.9	-2441.8
425.21	300	123.26	92.15	0.76	91.39	-2589.9	-2440.8
312.28	400	149.43	131.57	34.98	96.59	-2590.7	-2391
244.52	500	165.03	166.71	59.54	107.17	-2590.1	-2341.1
199.36	600	175.54	197.79	78.05	119.74	-2588.8	-2291.4
167.13	700	183.16	225.45	92.55	132.9	-2587.2	-2241.9
142.97	800	188.94	250.3	104.25	146.05	-2585.4	-2192.7
124.19	900	193.49	272.83	113.92	158.9	-2583.6	-2143.8
109.11	1000	197.16	293.41	122.07	171.34	-2603.1	-2093.5
96.73	1100	200.16	312.35	129.04	183.31	-2601.0	-2042.6
86.43	1200	202.67	329.88	135.07	194.8	-2598.8	-1992
77.72	1300	204.77	346.18	140.36	205.83	-2596.4	-1941.4
70.26	1400	206.56	361.43	145.02	216.4	-2594.1	-1891.2
63.8	1500	208.08	375.73	149.18	226.55	-2591.6	-1841.1
58.16	1600	209.38	389.2	152.9	236.3	-2589.2	-1791.1
53.17	1700	210.5	401.93	156.26	245.67	-2636.8	-1740.8
48.66	1800	211.46	413.99	159.3	254.69	-2634.1	-1688.2



LogKf	$\Delta H_{\text{andalusit-k}}$ (kJ/mol)	$\Delta c_p_{\text{andalusit-kyanit}}$ (J/mol K)
427.77	3.90	1.02
424.98	3.90	1.00
312.22	4.00	0.18
244.56	4.00	-0.22
199.48	3.90	-0.43
167.29	3.80	-0.54
143.17	3.80	-0.62
124.42	3.70	-0.66
109.35	3.70	-0.68
96.99	3.60	-0.69
86.71	3.50	-0.68
78.01	3.50	-0.67
70.56	3.40	-0.64
64.11	3.40	-0.62
58.47	3.30	-0.59
53.49	3.30	-0.56
48.99	3.20	-0.53

