High-Temperature Crystal Chemistry Of Danburite-Like Borosilicates

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Among unhydrous alkaline borosilicates $RB_2Si_2O_8$ (R = Ca, Sr, Ba) there are three naturally occurring members: danburite (Ca) (Dunbar, Machatschki, 1931), pekovite (Sr) and maleevite (Ba) (Pautov et al, 2004). Their orthorhombic structure consists of tetrahedral framework with boron and silicon orderly distributed in different tetrahedral sites. Almost all known unhydrous borosilicates are structurally similar to aluminosilicate relatives. Danburite structure type is topologically identical to that of paracelsian $RAl_2Si_2O_8$ (R = Sr, Ba), although the latter one represents pseudo-orthorhombic framework with monoclinity angle $\beta \sim 90.01°$

$CaB_2Si_2O_8$, danburite from Dalnegorsk, Russia
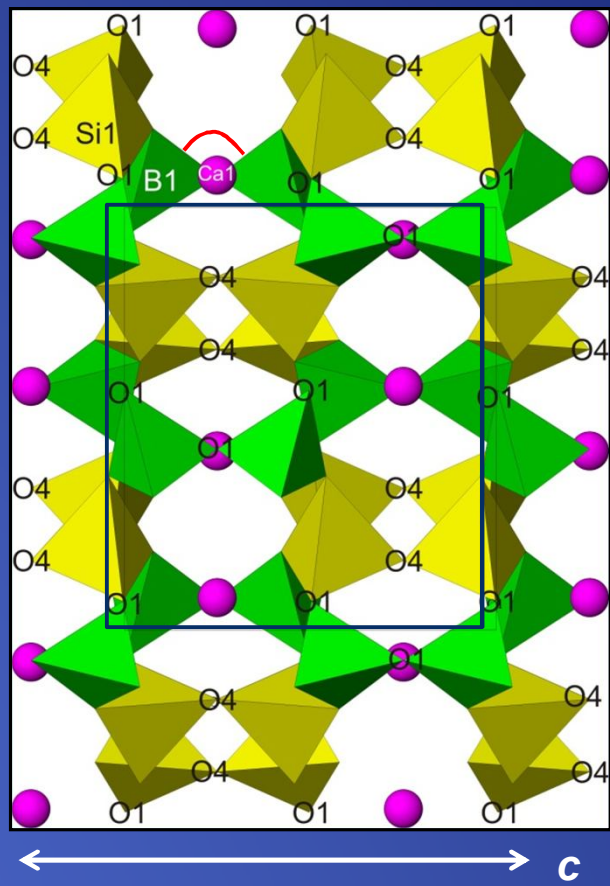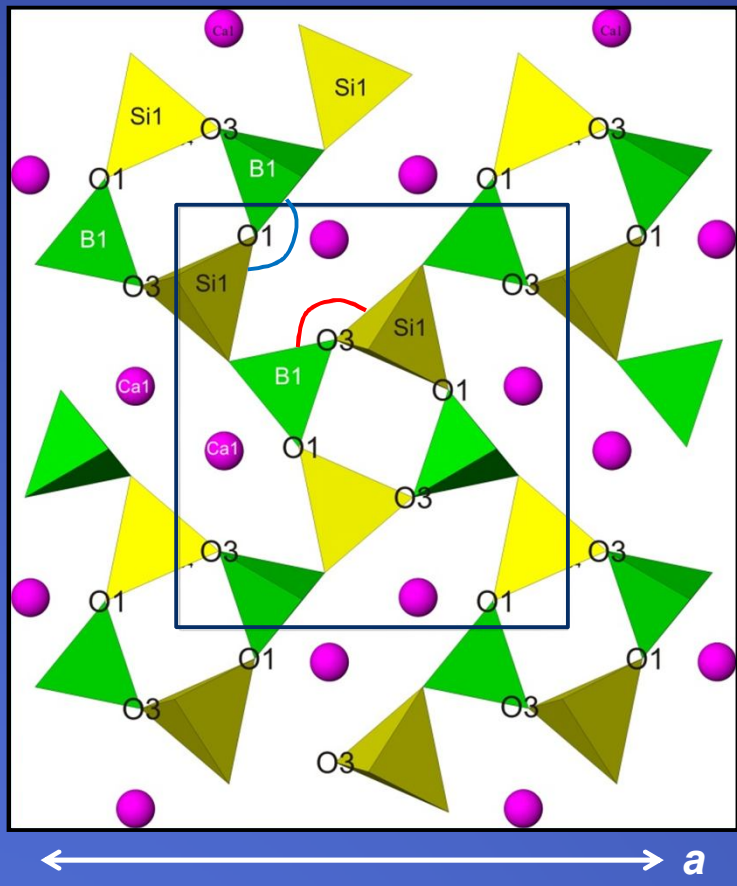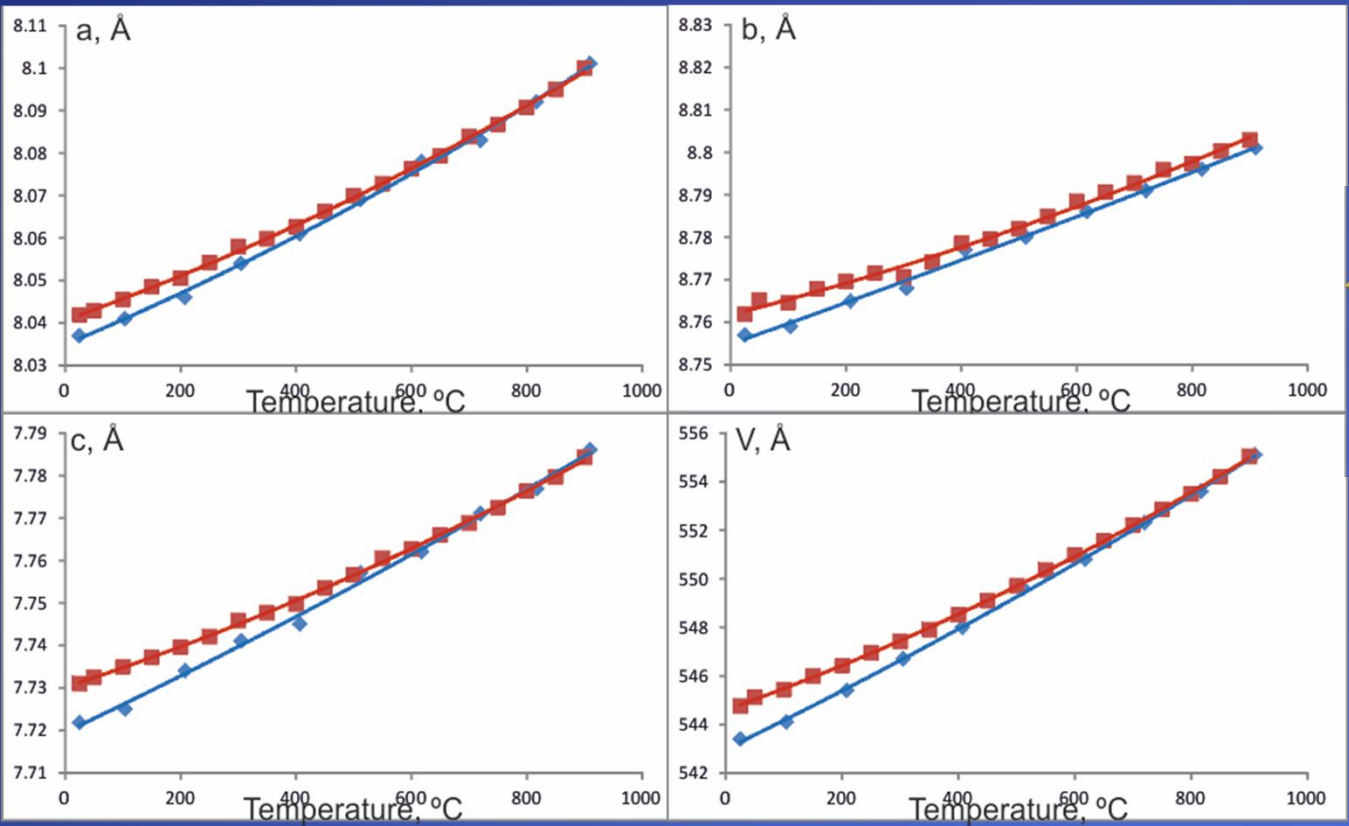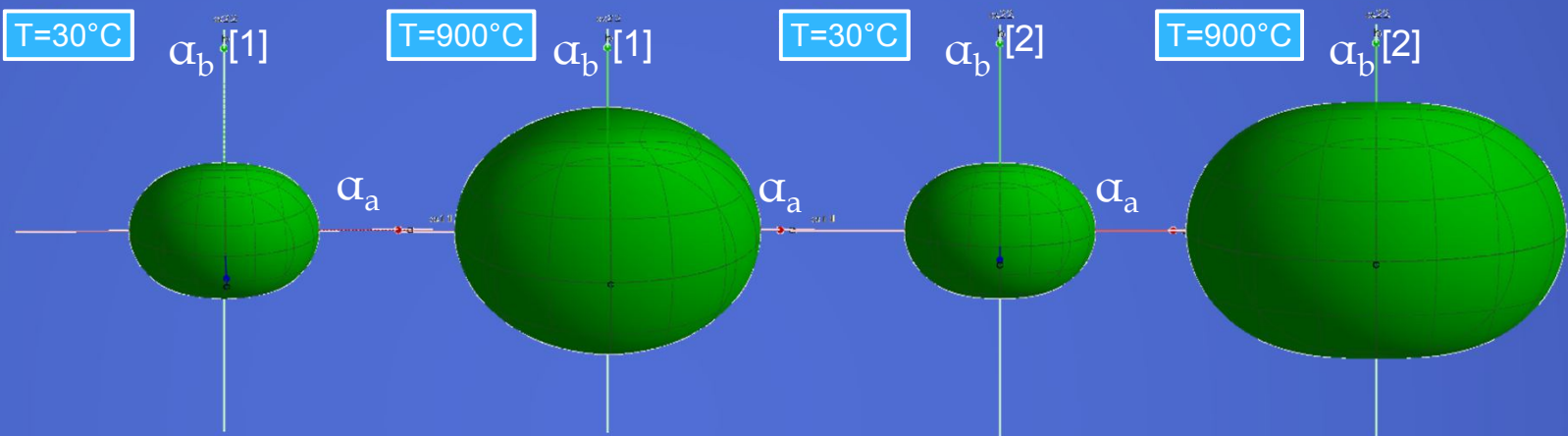

Structural changes of danburite on heating up to 1000 ºC [1]
Si-O(1)-B   - 0,64 °
Si-O(3)-B   1,45 °
Si-O(4)-Si   1,26 °
Ca-O(1)×2   0,05 Å
<Ca-O>₆ 0,03 Å

	30 °C		450 °C		900 °C	
	[1]	[2]	[1]	[2]	[1]	[2]
α_a	7	6	9	8	10	10
α_b	4	4	8	5	13	6
α_c	6	6	6	8	6	10
α_V	17	16	23	21	29	26

[1] K. Sugiyama, Y. Takeuchi, 1985   [2] Present work. Sample of danburite (Dalnegorsk, Primorie, Russia) is provided by Prof. I.V. Pekov
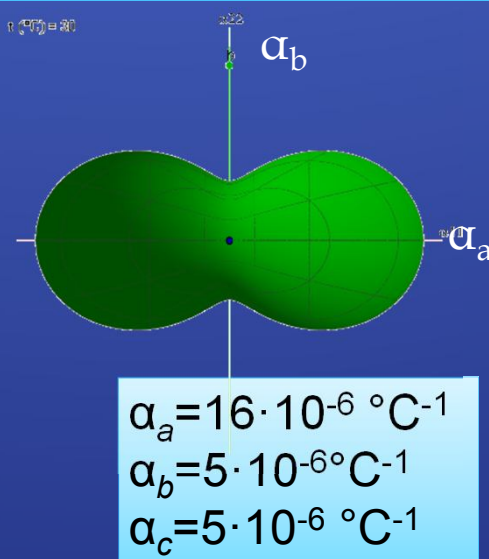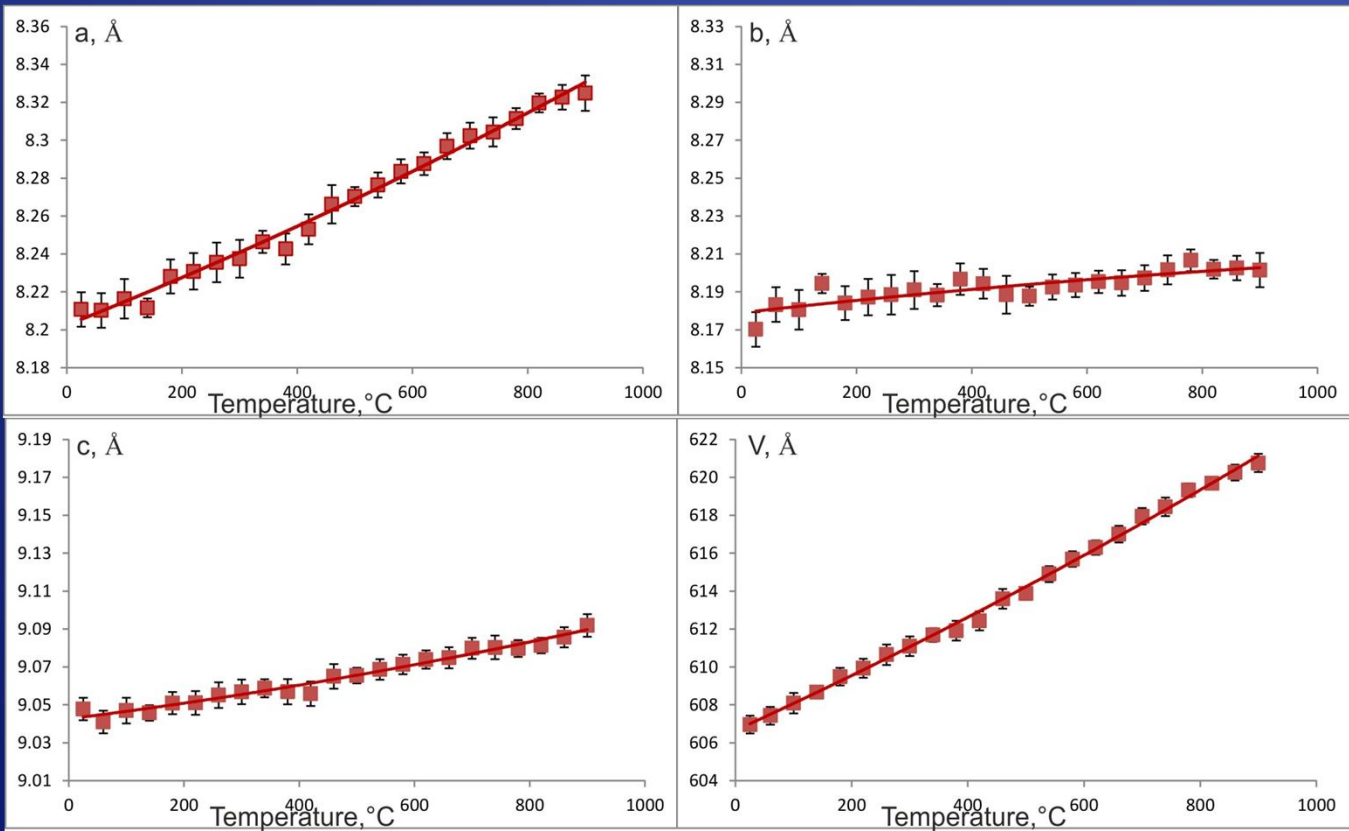
$SrB_2Si_2O_8$ prepared by solid state reactions at 900 ºC for 127 hours
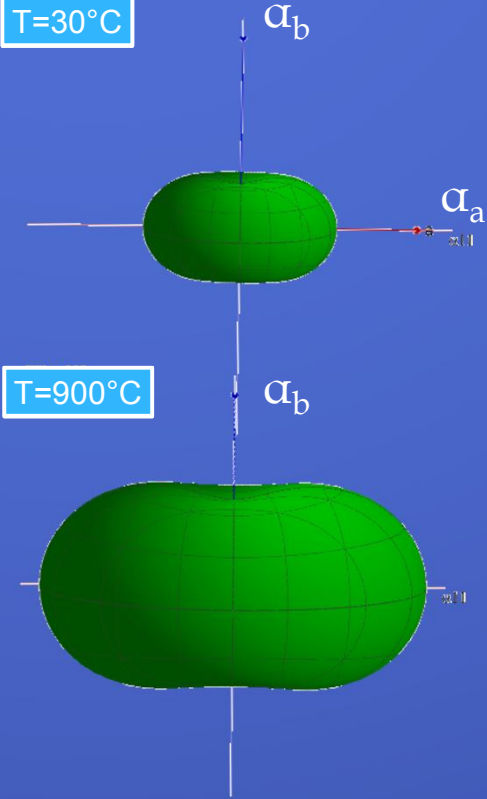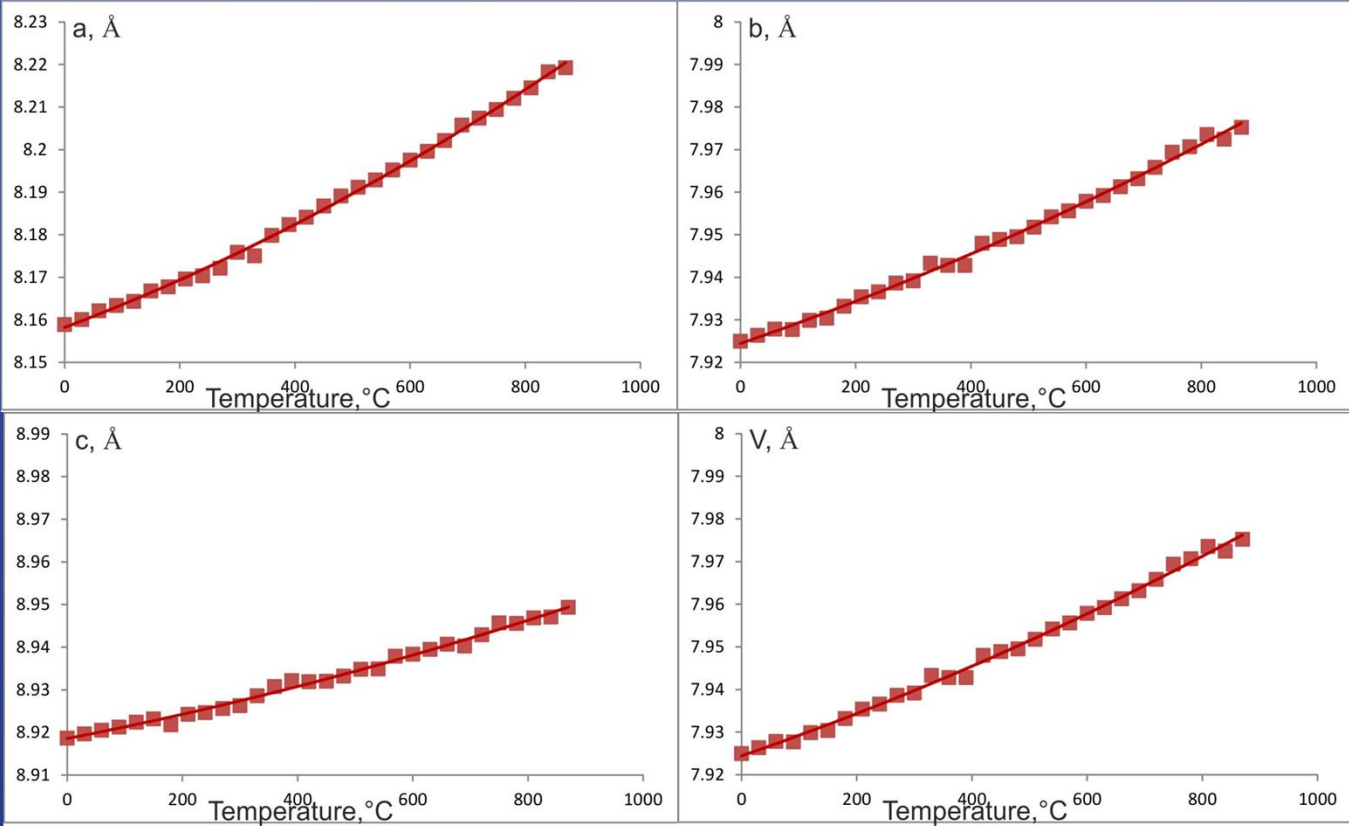
	30 °C	450 °C	900 °C
α_a	6	9	11
α_b	6	7	9
α_c	3	4	5
α_V	15	20	25
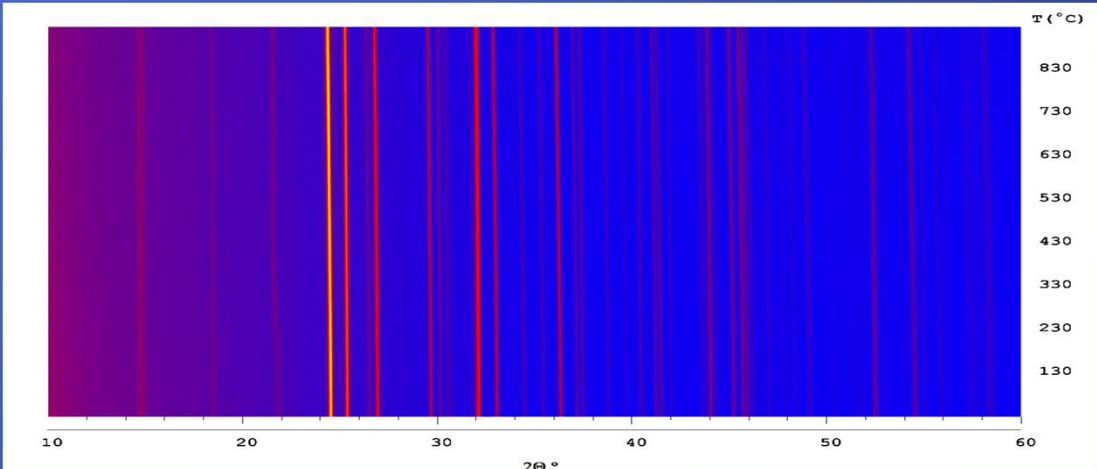
$BaB_2Si_2O_8$ prepared by cooling of stoichiometric melt from 1000 to 900 º C for 2.5 hours

$\alpha_a = 16 \cdot 10^{-6}$ °C^{-1}
$\alpha_b = 5 \cdot 10^{-6}$ °C^{-1}
$\alpha_c = 5 \cdot 10^{-6}$ °C^{-1}

Linear and volumetric thermal expansion coefficients for danburite–like $RB_2Si_2O_8$ (R = Ca, Sr, Ba) x10^6 °C^{-1}

	Ca	Ca*	Sr	Ba
α_a	7	9	9	16
α_b	5	8	7	5
α_c	7	6	4	5
α_V	19	23	20	23

* K. Sugiyama, Y. Takeuchi, 1985