J. Phase Equilib. Diffus. (2022) 43:266–273
https://doi.org/10.1007/s11669-022-00949-6

CORRECTION

Correction to: Phase Relations in the $CaO-B_2O_3-Sc_2O_3$ Ternary System

Wenke Zhi[1] · Xiaoyi Chen[1] · Fei Wang[1] · Yang Tian[1] · Yongnian Dai[1] · Bin Yang[1]

Published online: 21 April 2022

Correction to: J. Phase Equilib. Diffus. (2022) 43:98–108 https://doi.org/10.1007/s11669-021-00929-2

Note of changes: Abstract section

- "nonlinear optical" is modified to "nonlinear optical (NLO)"
- "systemically studied" is modified to "investigated comprehensively"
- "thermo dynamic" is modified to "thermodynamic"
- "electron probe microanalysis and x-ray diffraction" is modified to "electron probe microanalysis (EPMA) and X-ray diffraction (XRD)"

Note of changes: Introduction

"As the core devices of solid-state laser systems, nonlinear optical (NLO) materials can effectively expand the frequency range of commonly used laser sources and play an important role in the field of laser related science and technology, for example," is modified to "NLO materials, as the core devices of solid state laser systems, can effectively broaden the frequency range of commonly used laser sources and play an important role in the field of laser related science and technology, including". "However, the availability of lasers with different wavelengths is limited which requires exploration of new laser materials with other wave-lengths.[7] For an NLO material to be highly efficient it is important that it is phase matchable." is modified to "the availability of lasers with various wavelengths is restricted, necessitating the exploration of new laser materials with additional wavelengths.[7] It is critical for a NLO material to be phase matchable in order to be extremely efficient.[8]" "Since the second order (SO) NLO materials have excellent second-harmonic generation (SHG) capability, they have attracted much attention.[7] Up to now, a variety of NLO materials have been discovered, including borates, carbonates, and silicates.[9–16]" is modifed to "Due to the outstanding second-harmonic generation (SHG) capacity of second-order (SO) NLO materials, they have garnered considerable attention.[7] There have been several discoveries of NLO materials to date, including borates, carbonates and silicates.[9–16]"

- "complex" is modified to "complicated"
- "nonlinear optical (NLO)" is modified to "NLO"
- "second-harmonic generation (SHG)" is modified to "SHG"
- "Second-order" is modified to "SO"
- "The compounds $Ca_4LaO(BO_3)_3$[25], $Ca_4YO(BO_3)_3$[28], and $Ca_4GdO(BO_3)_3$[29], which are likely to be possible

The original article can be found online at https://doi.org/10.1007/s11669-021-00929-2.

✉ Fei Wang
fayerswing@hotmail.com

✉ Yang Tian
emontian@hotmail.com

Wenke Zhi
812103474@qq.com

[1] State Key Laboratory of Complex Nonferrous Metal Resources Clear Utilization, National Engineering Laboratory for Vacuum Metallurgy, Key Laboratory for Nonferrous Vacuum Metallurgy of Yunnan Province, Kunming University of Science and Technology, 650093 Yunnan, People's Republic of China

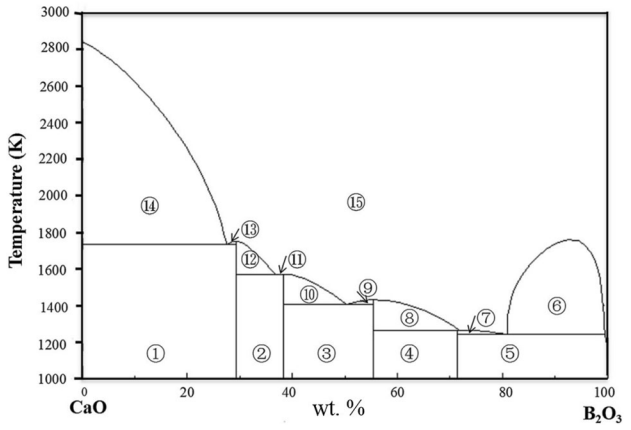

Fig. 1 Phase diagram in the system CaO-B_2O_3,[43] C=CaO, B=B_2O_3, L=Liquid. ① CaO+C_3B, ② C_2B+C_3B, ③ CB+C_2B, ④ CB+CB_2, ⑤ CB_2+L, ⑥ L+L1, ⑦ CB_2+L, ⑧ CB_2+L, ⑨ CB_2+L, ⑩ C_2B+L, ⑪ C_2B+L, ⑫ C_3B+L, ⑬ C_3B+L, ⑭ CaO+L, ⑮ L

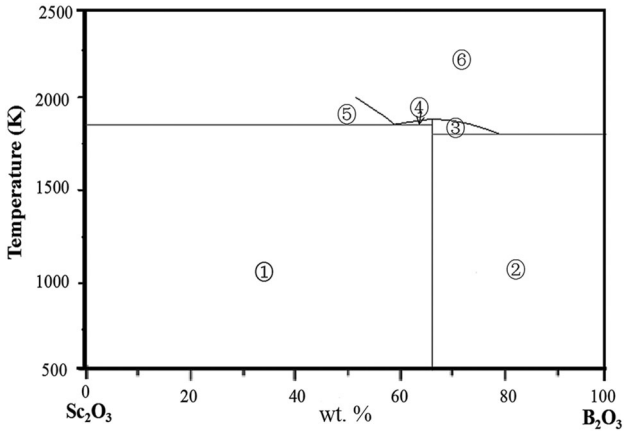

Fig. 2 Phase diagram in the system Sc_2O_3-B_2O_3.[44] ① Sc_2O_3+-$ScBO_3$, ② $ScBO_3$+L, ③ $ScBO_3$+L, ④ $ScBO_3$+L, ⑤ $ScBO_3$+L, ⑥ L"

good candidates for NLO materials." is modified to "$Ca_4LaO(BO_3)_3$[25], $Ca_4YO(BO_3)_3$ [28], and $Ca_4GdO(BO_3)_3$[29] are all compounds that are anticipated to be good candidates for NLO materials"

- "nonlinear optical" is modified to "NLO"

Note of changes: Experiment

- Experiment" is modified to "Experimental"
- "with 0.0001 g accuracy" is modified to "with a precision of 0.0001 g"
- "then the powder" is modified to "then filled with the powder"
- "after reaching the holding time it took 5 min to quench the samples." is modified to "the samples were to be quenched after the holding period had expired."
- "The samples were analyzed quantitatively by" is modified to "Quantitative analysis of the samples was done using"

Note of changes: Section 3.1.1

- "the $Ca_3B_2O_6$[39] $Ca_2B_2O_5$,[40] CaB_2O_4,[41] and CaB_4O_7[42] phases are found in the binary system CaO-B_2O_3.[43] $Ca_3B_2O_6$ (C_3B), CaB_2O_5 (C_2B) and CaB_2O_4 (CB) exist at 1373 K and C_3B and C_2B exist at 1473 K." is modified to "the $Ca_3B_2O_6$ (C_3B),[39] $Ca_2B_2O_5$ (C_2B),[40]CaB_2O_4 (CB),[41] and CaB_4O_7 (CB_2)[42] phases are found in the binary CaO-B_2O_3.[43] C_3B, C_2B and CB phases are existed at 1373 K and C_3B and C_2B phases are existed at 1473 K."

Note of changes: Section 3.1.2

"there is only $ScBO_3$[45] which exists at 1373 K and 1473 K." is modified to "there is only $ScBO_3$[45] existed at 1373 K and 1473 K."

Note of changes: Section 3.2.1

"The different chemical compositions of all phases result in different brightness in the grayscale image of the micrographs and, therefore, these phases can be distinguished easily." is modified to "Because of the various chemical compositions of each phase, the grayscale micrographs show a distinct difference in brightness, making it easy to identify between them."

- "C_3-B" is modified to "C_3-B"
- "Ca_4-$ScO(BO_3)_3$" is modified to "Ca_4-$ScO(BO_3)_3$"
- "Ca_3-$Sc_2(BO_3)_4$" is modified to "Ca_3-$Sc_2(BO_3)_4$"
- "C_2-B" is modified to "C_2-B"

Note of changes: Section 3.2.2

- "Fig. 4 and 5" is modified to " Figs. 4 and 5"
- "C_2B+ $Ca_3Sc_2(-BO_3)_4$+L" is modified to "C_2B+ Ca_3-$Sc_2(BO_3)_4$+L"
- "According to the lever,[47]" is modified to "According to the lever rule,[47]"
- "strongly" is modified to "substantially"

Note to changes: Section 3.3

- "Ca_4-$ScO(BO_3)_3$" is modified to "Ca_4-$ScO(BO_3)_3$"
- "So" is modified to "Accordingly"
- "found" is modified to "discovered"

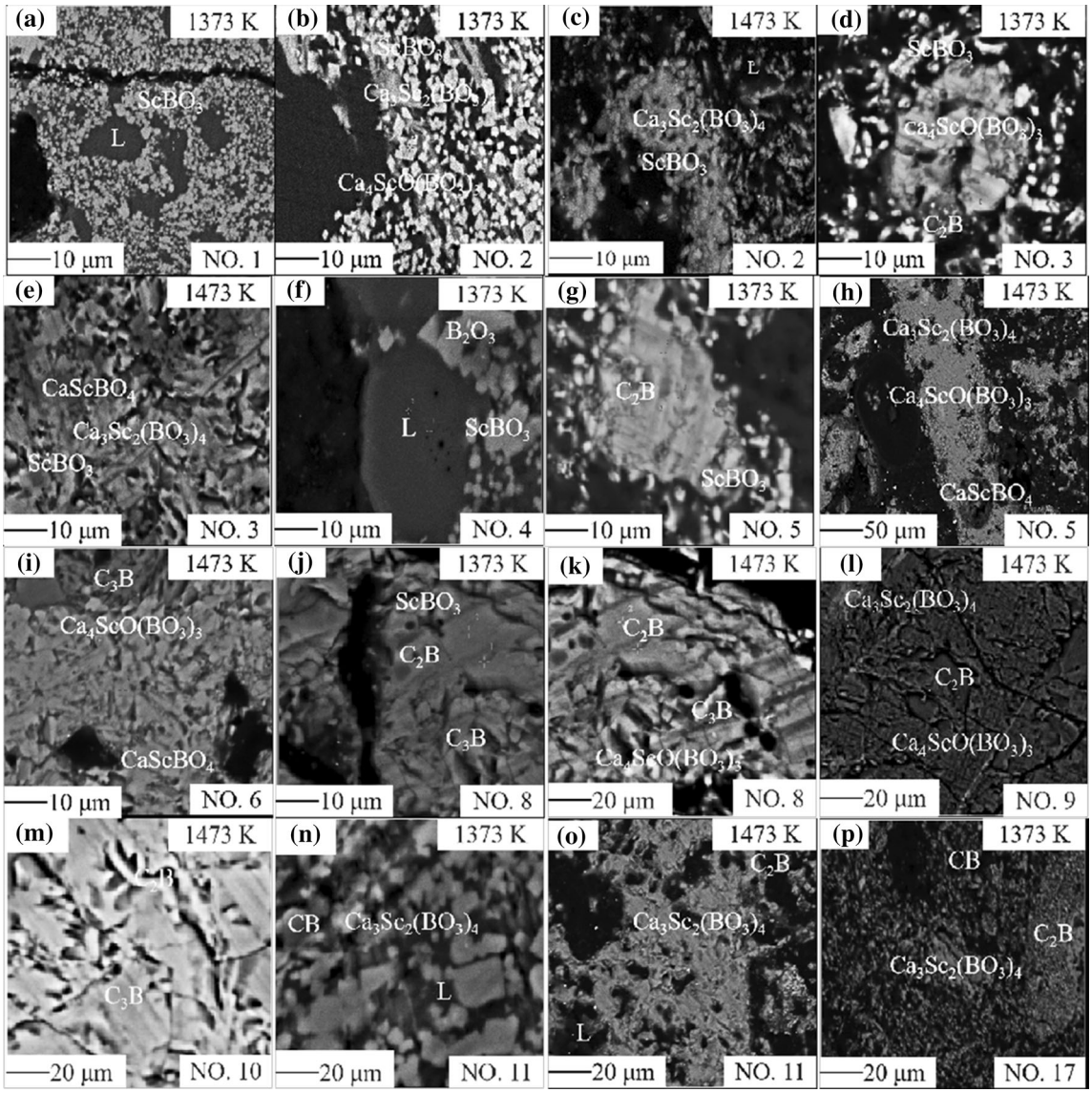

Fig. 3 Microstructures of the quenched slag samples. (a) $ScBO_3$ in equilibrium with L; (b) $Ca_3Sc_2(BO_3)_4$, $ScBO_3$ and $Ca_4ScO(BO_3)_3$ in equilibrium; (c) $Ca_3Sc_2(BO_3)_4$ and $ScBO_3$ in equilibrium with L; (d) C_2B (Sc_2O_3), $ScBO_3$ and $Ca_4ScO(BO_3)_3$ in equilibrium; "I" is modified to "(e)" $CaScBO_4$, $Ca_3Sc_2(BO_3)_4$ and $ScBO_3$ in equilibrium; (f) B_2O_3 and $ScBO_3$ in equilibrium with L; (g) C_2B (Sc_2O_3) and $ScBO_3$ in equilibrium; (h) $CaScBO_4$, $Ca_3Sc_2(BO_3)_4$ and $Ca_4ScO(BO_3)_3$ in equilibrium; (i) $CaScBO_4$, $Ca_4ScO(BO_3)_3$ and C_3B (Sc_2O_3) in equilibrium; (j) C_2B (Sc_2O_3), C_3B (Sc_2O_3) and $ScBO_3$ in equilibrium; (k) C_2B (Sc_2O_3), C_3B (Sc_2O_3) and $Ca_4ScO(BO_3)_3$ in equilibrium; (l) C_2B (Sc_2O_3), $Ca_4ScO(BO_3)_3$ and $Ca_3Sc_2(BO_3)_4$ in equilibrium; (m) C_2B (Sc_2O_3) and C_3B (Sc_2O_3) in equilibrium; (n) CB (Sc_2O_3) and $Ca_3Sc_2(BO_3)_4$ in equilibrium with L; (o) C_2B (Sc_2O_3) and $Ca_3Sc_2(BO_3)_4$ in equilibrium with L; (p) CB (Sc_2O_3), C_2B (Sc_2O_3) and $Ca_3Sc_2(BO_3)_4$ in equilibrium

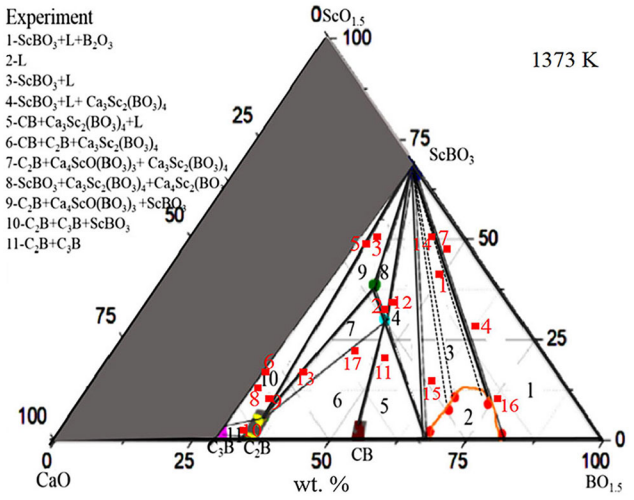

Fig. 4 Isothermal phase diagram of B_2O_3-Sc_2O_3-CaO system at 1373 K

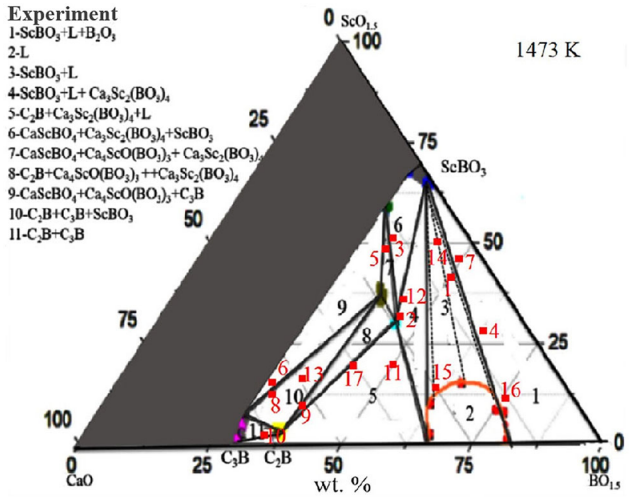

Fig. 5 Isothermal phase diagram of B_2O_3-Sc_2O_3-CaO system at 1473 K

- "The electron exchange correlation functions are calculated using" is modified to "The electron exchange correlation functions are calculated using"
- "The calculated results are consistent with the experimental results. The experimental results are shown in Fig. 9 and 10. The calculated results are consistent with the experimental results." is modified to "There is no discrepancy between the calculated and experimental results. Figs. 9 and 10 demonstrate the experimental results. There is agreement between the calculated and experimental results."
- "Fig. 9 and 10" is modified to "Figs. 9 and 10"

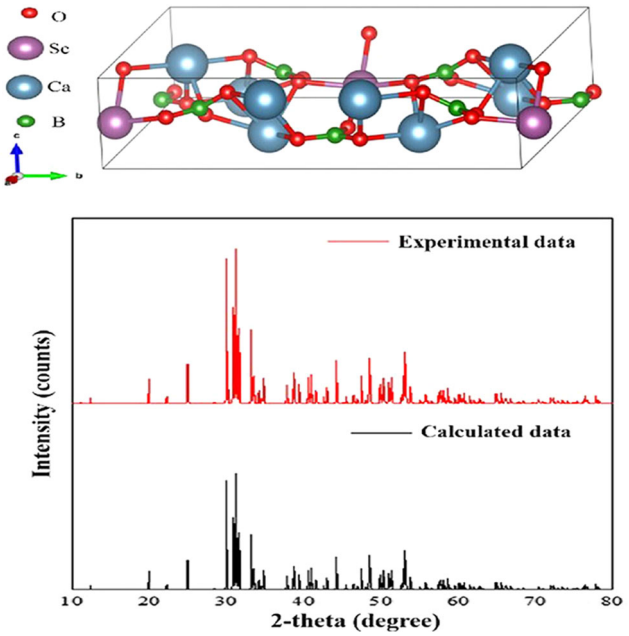

Fig. 6 (a) Crystal structure of $Ca_4ScO(BO_3)_3$ (b) Experimental and calculated XRD patterns of $Ca_4ScO(BO_3)_3$

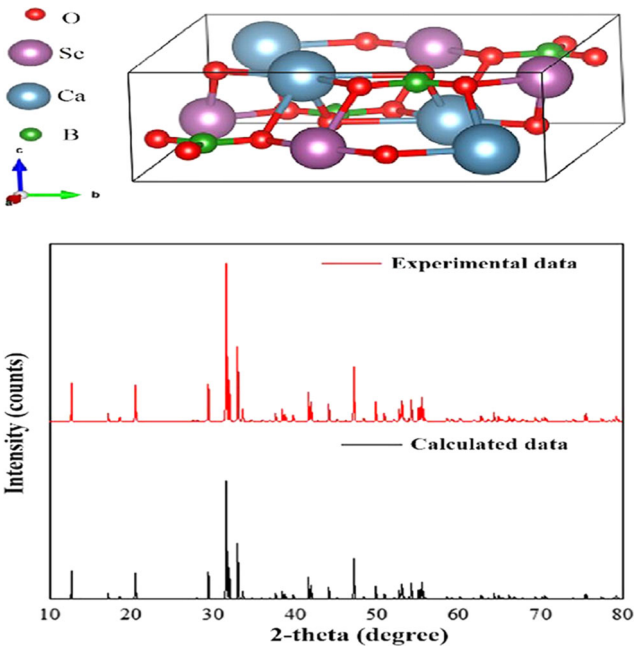

Fig. 7 (a) Crystal structure of $CaScBO_4$ (b) Experimental and calculated XRD patterns of $CaScBO_4$

Note of changes: Conclusions

"The data could also be used for theoretical calculations to understand and describe the ternary CaO-B_2O_3-Sc_2O_3 system." is modified to "Also, theoretical calculations

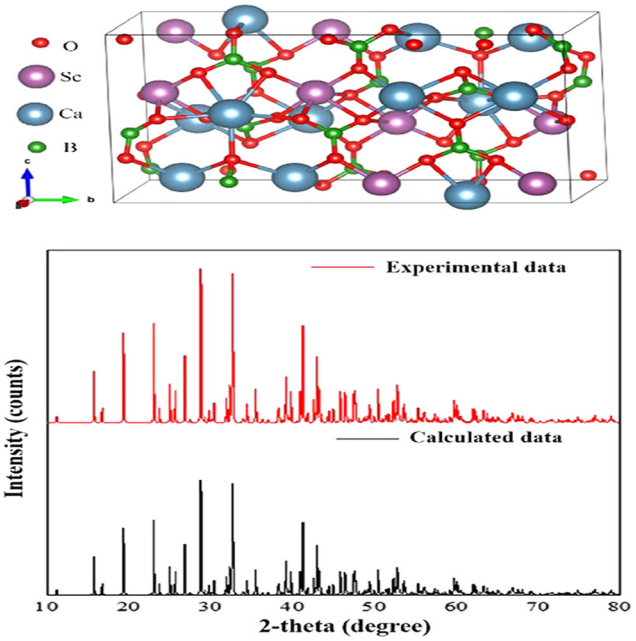

Fig. 8 (a) Crystal structure of $Ca_3Sc_2(BO_3)_4$ (b) Experimental and calculated XRD patterns of $Ca_3Sc_2(BO_3)_4$

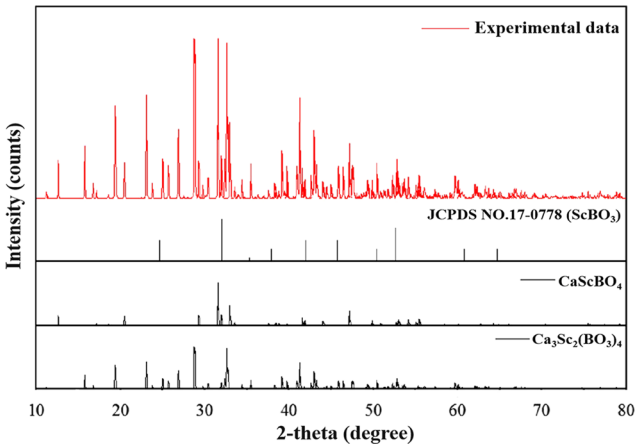

Fig. 9 XRD patterns of the $CaScBO_4$, $Ca_3Sc_2(BO_3)_4$ and $ScBO_3$

based on the data might be employed in an effort to better comprehend and explain the ternary CaO-B_2O_3-Sc_2O_3 system."

Note of changes: The title of Fig. 1 is modified as follows:

Fig. 1 Phase diagram in the system CaO-B_2O_3.[43] C=CaO, B=B_2O_3. ① CaO+$Ca_3B_2O_6$, ② $Ca_2B_2O_5$+$Ca_3B_2O_6$, ③ CaB_2O_4+$Ca_2B_2O_5$, ④ CaB_2O_4+CaB_4O_7, ⑤ CaB_4O_7+Liquid, ⑥ Liquid+Liquid1, ⑦ CaB_4O_7+Liquid, ⑧ CaB_2O_4+Liquid, ⑨ CaB_2O_4+Liquid, ⑩ $Ca_2B_2O_5$+Liquid, ⑪ $Ca_2B_2O_5$+ Liquid, ⑫ $Ca_3B_2O_6$+ Liquid, ⑬ $Ca_3B_2O_6$+Liquid, ⑭ CaO+Liquid, ⑮ Liquid" is modified to "**Fig. 1** Phase diagram in the system CaO-B_2O_3,[43] C=CaO, B=B_2O_3, L=Liquid. ① CaO+C_3B, ② C_2B+ C_3B, ③ CB+C_2B, ④ CB+CB_2, ⑤ CB_2+L, ⑥ L + L1, ⑦ CB_2+ L, ⑧ CB_2+L, ⑨ CB_2+L, ⑩ C_2B+L, ⑪ C_2B+ L, ⑫ C_3B+L, ⑬ C_3B+L, ⑭ CaO+L, ⑮ L. In addition, "wt %" is modified to "wt.%" in the Fig. 1.

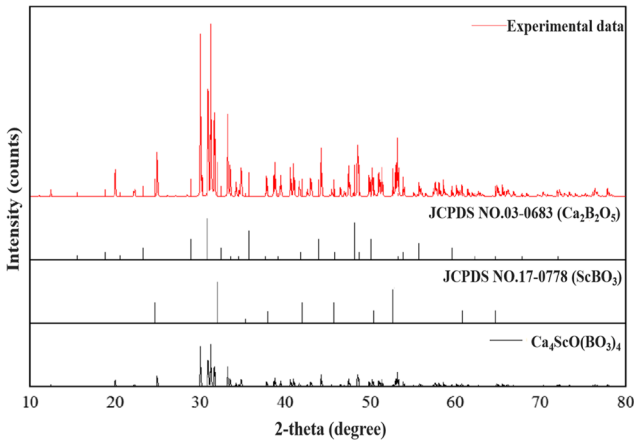

Fig. 10 XRD patterns of the $Ca_4ScO(BO_3)_3$, $Ca_2B_2O_5$ and $ScBO_3$

Table 1 Initial compositions (wt. %) for the system CaO-B_2O_3-Sc_2O_3 at 1373 K and 1473 K

No.	B_2O_3	Sc_2O_3	CaO	No.	B_2O_3	Sc_2O_3	CaO
1	50.00	39.97	9.99	10	29.00	2.99	57.94
2	40.00	29.98	29.96	11	50.00	19.99	29.96
3	30.00	49.97	19.97	12	40.00	34.98	24.98
4	62.00	27.98	9.99	13	35.00	16.99	46.95
5	28.00	49.97	26.97	14	40.00	49.97	9.99
6	29.00	14.99	55.95	15	60.00	14.99	24.98
7	47.00	44.97	7.99	16	75.00	9.99	14.99
8	30.00	11.99	57.94	17	40.00	19.99	39.96
9	34.00	8.99	56.94	.	.	.	.

Note of changes: The title of Fig. 2 is modified as follows:

"**Fig. 2** Phase diagram in the system Sc_2O_3-B_2O_3.[44] ① Sc_2O_3+$ScBO_3$, ② $ScBO_3$+L, ③ $ScBO_3$+L, ④ $ScBO_3$+L, ⑤ Sc_2BO_3+L, ⑥ L". In addition, "wt %" is modified to "wt. %" in the Fig. 2.

Note of changes: The temperature (1373 K or 1473 K) is added and the order (from small to large) is changed in Fig. 3. The modified result is as follows:

Note of changes: "wt %" is modified to "wt. %" in the Figs. 4 and 5. The modified results are as follows:

Note of changes: "Calculative data" is modified to "Calculated data" in Figs. 6-8. The boxes on the "Calculated data" and "Experimental data" are removed in Figs. 6-8. The modified results are as follows:

Note of changes: The boxes on the "Experimental data", "JCPDS NO.17-0778

Table 2 Phase relations and compositions in the systems CaO-B_2O_3-Sc_2O_3 at 1373 K and 1473 K

Nominal composition No. wt. %		Observed phase(s)	
		1373 K	1473 K
1	$50B_2O_3$-$39.97Sc_2O_3$-9.99CaO	$ScBO_3$+L	L+$ScBO_3$
2	$40B_2O_3$-$29.98Sc_2O_3$-29.96CaO	$Ca_3Sc_2(BO_3)_4$+$Ca_4ScO(BO_3)$+$ScBO_3$	L+$ScBO_3$+$Ca_3Sc_2(BO_3)_4$
3	$30B_2O_3$-$49.97Sc_2O_3$-19.97CaO	C_2B+$ScBO_3$+$Ca_4ScO(BO_3)_3$	$CaScBO_4$+$Ca_3Sc_2(BO_3)_4$ +$ScBO_3$
4	$62B_2O_3$-$27.98Sc_2O_3$-9.99CaO	$ScBO_3$+L+B_2O_3	$ScBO_3$+B_2O_3+L
5	$28B_2O_3$-$49.97Sc_2O_3$-26.97CaO	$ScBO_3$+C_2B	$Ca_4ScO(BO_3)_3$+$CaScBO_4$ +$Ca_3Sc_2(BO_3)_4$
6	$29B_2O_3$-$14.99Sc_2O_3$-55.95CaO	$ScBO_3$+C_2B+C_3B	C_3B+$Ca_4ScO(BO_3)_3$+$CaScBO_4$
7	$47B_2O_3$-$44.97Sc_2O_3$-7.99CaO	$ScBO_3$+L+B_2O_3	$ScBO_3$+L+B_2O_3
8	$30B_2O_3$-$11.99Sc_2O_3$-57.94CaO	$ScBO_3$+C_2B+C_3B	$Ca_4ScO(BO_3)_3$+C_2B+C_3B
9	$34B_2O_3$-$8.99Sc_2O_3$-56.94CaO	$ScBO_3$+C_2B	C_2B+$Ca_4ScO(BO_3)_3$+$Ca_3Sc_2(BO_3)_4$
10	$29B_2O_3$-$2.99Sc_2O_3$-57.94CaO	C_2B+C_3B	C_2B+C_3B
11	$50B_2O_3$-$19.99Sc_2O_3$-29.96CaO	CB+$Ca_3Sc_2(BO_3)_4$+L	L+C_2B+$Ca_3Sc_2(BO_3)_4$
12	$40B_2O_3$-$34.98Sc_2O_3$-24.98CaO	$ScBO_3$+L+$Ca_3Sc_2(BO_3)_4$	L+$ScBO_3$+$Ca_3Sc_2(BO_3)_4$
13	$35B_2O_3$-$16.99Sc_2O_3$-46.95CaO	C_2B+$Ca_4ScO(BO_3)_3$ +$Ca_3Sc_2(BO_3)_4$	C_2B+C_3B+$Ca_4ScO(BO_3)_3$
14	$40B_2O_3$-$49.97Sc_2O_3$-9.99CaO	$ScBO_3$+L	$ScBO_3$+L
15	$60B_2O_3$-$14.99Sc_2O_3$-24.98CaO	$ScBO_3$+L	$ScBO_3$+L
16	$75B_2O_3$-$9.99Sc_2O_3$-14.99CaO	$ScBO_3$+L+B_2O_3	$ScBO_3$+L+B_2O_3
17	$40B_2O_3$-$19.99Sc_2O_3$-39.96CaO	CB+C_2B+$Ca_3Sc_2(BO_3)_4$	C_2B+$Ca_3Sc_2(BO_3)_4$+L

Table 3 Calculated structural parameters from powder X-ray analysis of $Ca_4ScO(BO_3)_3$ for space group Cm, a=9.0268 Å, b=9.0268 Å, and c=3.5647 Å

Atom	x	y	z
Ca	0.67030	− 0.55712	0.72206
Ca	0.12603	− 0.23257	0.04655
B	0.06375	− 0.55059	0.46999
B	0.82603	− 0.17397	0.11470
Sc	0.19645	− 0.80355	0.35654
O	0.99303	− 0.73748	0.46898
O	0.81467	− 0.33477	0.13924
O	0.95995	− 0.50669	0.66959
O	0.24010	− 0.40583	0.27184
O	0.34831	− 0.65169	0.82974
O	− 0.00007	− 1.00007	0.06342

Table 4 Selected bond distances (Å) in $Ca_4ScO(BO_3)_3$

Bonds	Length	Bonds	Length
Ca-O11	2.394	O8-Ca2	2.412
Ca-O11	2.387	O8-Ca2	2.397
Ca-O14	2.359	O8-B6	1.406
Ca-O16	2.369	O11-B5	1.387
Ca-O16	2.303	O11-Ca2	2.359
Ca2-O8	2.412	O11-Ca	2.387
Ca2-O8	2.397	O14-B6	1.384
Ca2-O11	2.359	O16-Ca	2.369
B6-O14	1.384	O16-Ca	2.303
B6-O16	1.383	O10-Sc4	2.037
B6-O8	1.406	O13-B5	1.391
B5-O11	1.387	Sc4-O10	2.037
B5-O13	1.391	Sc4-O13	2.074

Table 5 Calculated structural parameters from powder X-ray analysis of $CaScBO_4$ for space group Pnma, a=10.3449 Å, b=3.386 Å, and c=9.57 Å

Atom	x	y	z
Ca	0.58887	0.25	0.65998
Sc	0.60999	0.25	0.06956
B	0.69364	0.25	0.36395
O	0.76596	0.25	0.48747
O	0.75451	0.25	0.23410
O	0.56078	0.25	0.37495
O	1.00041	0.25	0.61442

Table 6 Selected bond distances (Å) in $CaScBO_4$

Bonds	Length	Bonds	Length
Ca-O12	2.466	B8-O16	1.393
Ca-O24	2.345	B8-O20	1.378
Sc4-O16	2.171	O24-Sc4	2.087
Sc4-O24	2.087	O24-Sc4	2.087
Sc4-O24	2.087	O24-Sc4	2.094
Sc4-O24	2.094	O24-Ca	2.345
B8-O12	1.399	.	.

($ScBO_3$)", "$CaScBO_4$" and "$Ca_3Sc_2(BO_3)_4$" are removed in Fig. 9. The modified result is as follows:

Note of changes: The boxes on the "Experimental data", "JCPDS NO.17-0778 ($ScBO_3$)", "JCPDS NO. 03-0683 ($Ca_2B_2O_5$)", "$CaScBO_4$" and "$Ca_3Sc_2(BO_3)_4$" are removed in Fig. 10. The modified result is as follows:

Note of changes: The modified results of Tables 1-5 (three-line tables) are as follows:

Table 7 Calculated structural parameters from powder X-ray analysis of $Ca_3Sc_2(BO_3)_4$ for space group Pnma, a=7.123 Å, b=15.633 Å, and c=9.1764 Å

Atom	x	y	z
Ca	0.18498	0.12675	− 0.60954
Sc	0.40493	0.57967	− 0.60212
B	0.30802	0.47223	− 0.88863
O	0.13014	0.52105	− 0.24899
O	− 0.3266	0.97290	− 0.55089
O	0.13553	0.90700	− 0.48142
O	0.49121	0.82721	− 0.44115
O	0.31674	0.82558	− 0.73055
Ca	− 0.20234	0.25000	− 0.49506
B	− 0.04928	0.25000	− 0.88083
B	− 0.33892	0.25000	− 0.19129
O	− 0.17372	0.25000	− 0.76456
O	0.38125	0.75000	− 0.95618

Table 8 Selected bond distances (Å) in $Ca_3Sc_2(BO_3)_4$

Bonds	Length	Bonds	Length
Ca4-Ca	3.525	O72-Ca	2.159
Ca4-O49	2.432	O72-B25	1.391
Ca4-O36	3.075	Ca-Ca4	3.525
Ca4-O36	2.470	Ca-Sc12	3.157
Sc12-Ca	3.157	Ca-Sc12	3.157
Sc12-O56	2.163	Ca-O40	2.481
Sc12-O36	2.088	Ca-O49	2.315
Sc12-O37	2.134	Ca-O56	2.456
B20-O41	1.388	Ca-O56	2.456
B20-O36	1.359	Ca-O72	2.519
B20-O37	1.401	Ca-O72	2.519
O36-Ca4	2.470	B21-O40	1.387
O36-Ca4	3.075	B21-O56	1.391
O36-B20	1.359	B21-O56	1.391
O36-Sc12	2.088	B25-O49	1.386
O37-B20	1.401	B25-O72	1.391
O37-Sc12	2.134	B25-O72	1.391
O41-B20	1.388	O49-Ca4	2.432
O56-Ca	2.456	O49-Ca4	2.432
O56-Sc12	2.163	O49-Ca	2.315
O56-B21	1.391	O49-B25	1.386

Note of changes: "Y" is modified to "Sc", and the modified results of Table 6 (three-line tables) are as follows:

Note of changes: The modified results of Tables 7-8 (three-line tables) are as follows:

Note of changes: Reference Section

- Reference "19. M. Mutailipu, M. Zhang, X. Su, Z. Yang, Y. Chen, and S. Pan, Structural Insights into Borates with an Anion-Templated OpenFramework Configuration: Asymmetric K2BaB16O26 versus Centrosymmetric K3CsB20O32 and Na2M2NB18O30 (M=Rb, Cs;N= Ba, Pb), *Chem. Eur. J.,* 2017, **23**, p 13910–13918." is modified to "19. M. Mutailipu, M. Zhang, X. Su, Z. Yang, Y. Chen, and S. Pan, Structural Insights into Borates with an Anion-Templated Open-Framework Configuration: Asymmetric $K_2BaB_{16}O_{26}$ versus Centrosymmetric $K_3CsB_{20}O_{32}$ and $Na_2M_2NB_{18}O_{30}$ (M=Rb, Cs; N=Ba, Pb), *Chem. Eur. J.,* 2017, **23**, p 13910–13918."
- Reference "24. H.Y.-P. Hong, and K. Dwight, Crystal Structure and Fluorescence Lifetime of NdAl3 (BO3) 4, A Promising Laser Material, *Mater. Res. Bull.,* 1974, **9**, p 1661–1665. https://doi.org/10.1016/0025-5408(74)90158-5" is modified to "24. H.Y.-P. Hong, and K. Dwight, Crystal Structure and Fluorescence Lifetime of $NdAl_3(BO_3)_4$, A Promising Laser Material, Mater. Res. Bull., 1974, **9**, p 1661–1665. https://doi.org/10.1016/0025-5408(74)90158-5."