A Series of Boroselenite-based Open Frameworks Mediated by The Cationic Sizes of the Alkali Metals

Jian-Han Zhang, Fang Kong, Bing-Ping Yang, and Jiang-Gao Mao*

Supporting Information

Figure S1. The energy-dispersive spectrometry plots and ratios for $NaSeB_3O_7$ (a), $KSeB_3O_7$ (b) and $K_2Se_3B_2O_{10}$ (c).

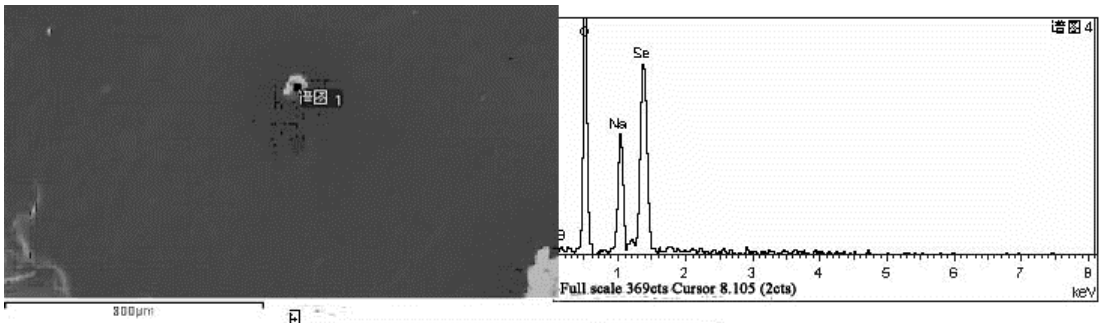
Figure S2. Simulated and measured XRD powder patterns for $Li_2SeB_8O_{15}$ (a), $NaSeB_3O_7$ (b), $KSeB_3O_7$ (c), and $K_2Se_3B_2O_{10}$ (d).

Figure S3. a) View of the structure of $NaSeB_3O_7$ along *a*-axis. b) Side view of $[SeB_3O_7]^-$ layer with 10-MRs channels along c-axis. c) The 10-MR with a free diameter of 6.91× 4.47 Å. d) View of the structure of $NaSeB_3O_7$ along *c*-axis. Na, Se, B, and O atoms are drawn as green, pink, yellow, and red circles, respectively.

Figure S4. a) View of the structure of $Li_2SeB_8O_{15}$ along *a*-axis. b) A 2D anionic borate layer of $[B_4O_{18}]^{4-}$ in *ac* plane. c) A single $[SeB_8O_{15}]^{2-}$ framework with large 14- and 16-MRs channels along *c*-axis. d) 2-fold interpenetrating $[SeB_8O_{15}]^{2-}$ anionic frameworks. Li, Se, B, and O atoms are drawn as green, pink, yellow, and red circles, respectively.

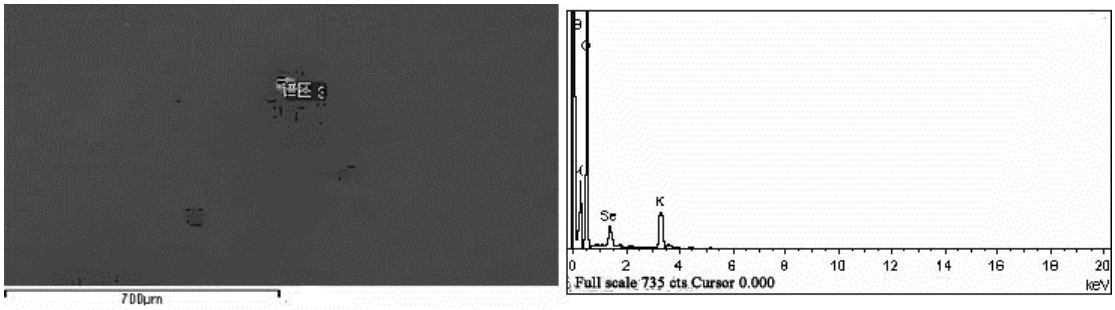
Figure S5. Optical diffuse reflectance spectra for $Li_2SeB_8O_{15}$ (a), $NaSeB_3O_7$ (b), $KSeB_3O_7$ (c), and $K_2Se_3B_2O_{10}$ (d).

Figure S6. IR spectra for $Li_2SeB_8O_{15}$ (a), $NaSeB_3O_7$ (b), $KSeB_3O_7$ (c), and $K_2Se_3B_2O_{10}$ (d).



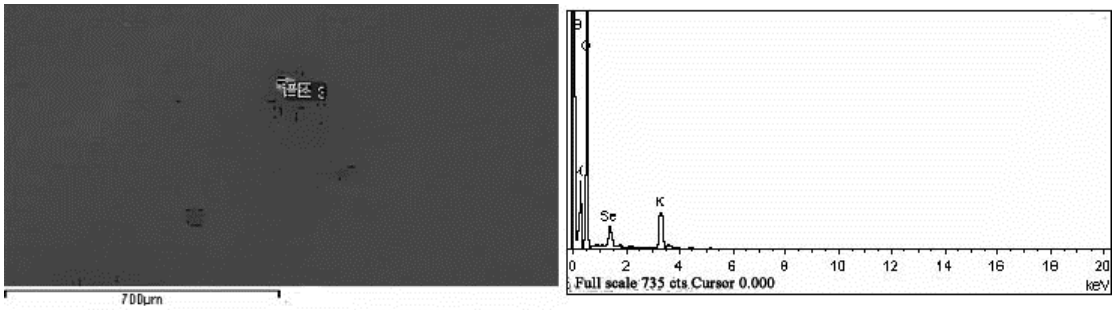
Element	Weight (%)	Atoms (%)
Na	8.95	7.82
Se	25.6	6.52

(a)



Element	Weight (%)	Atoms (%)
K	13.82	8.02
Se	25.45	7.29

(b)



Element	Weight (%)	Atoms (%)
K	13.82	8.02
Se	25.45	7.29

(c)

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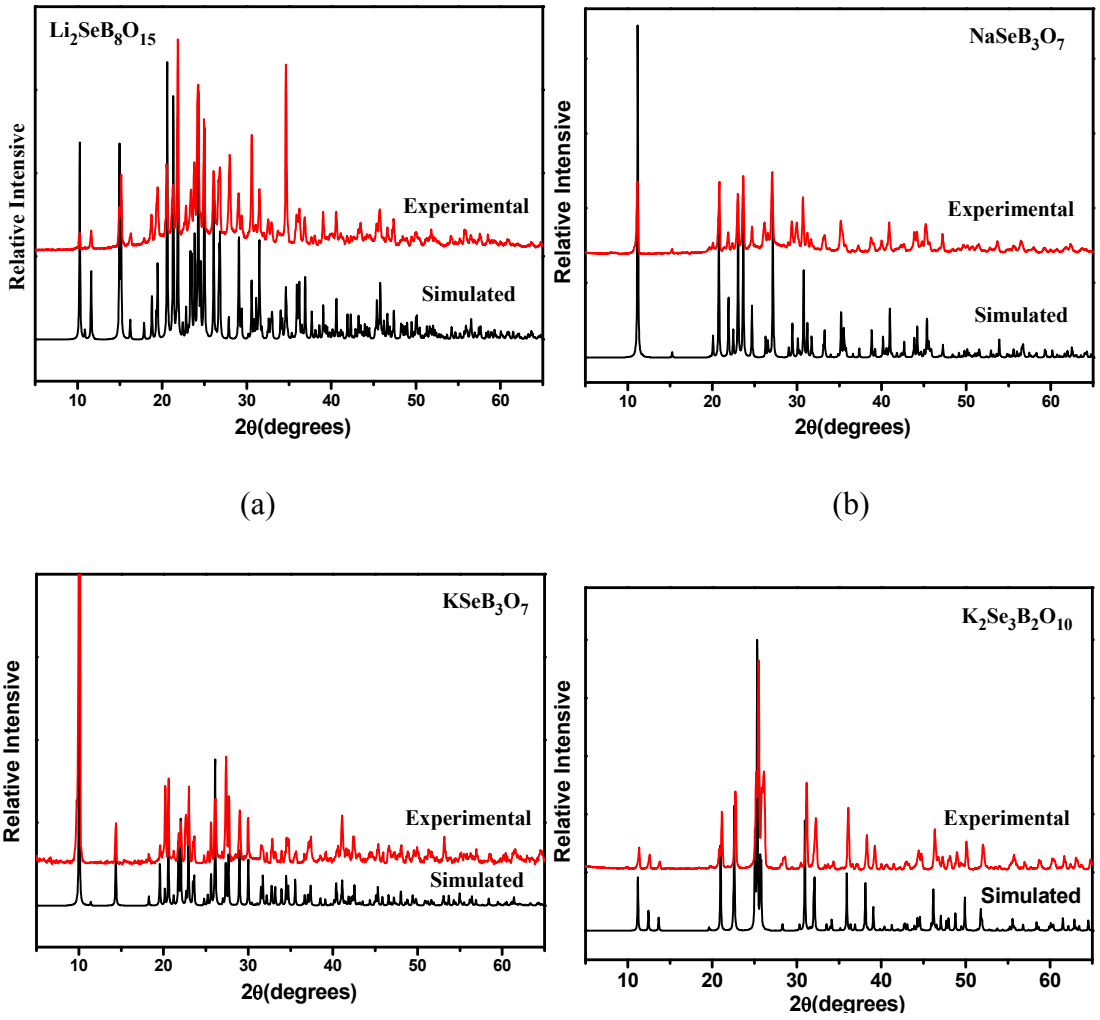

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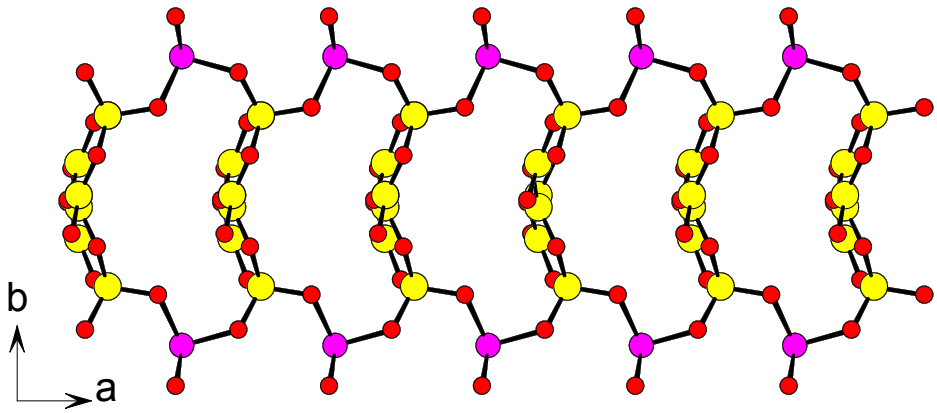
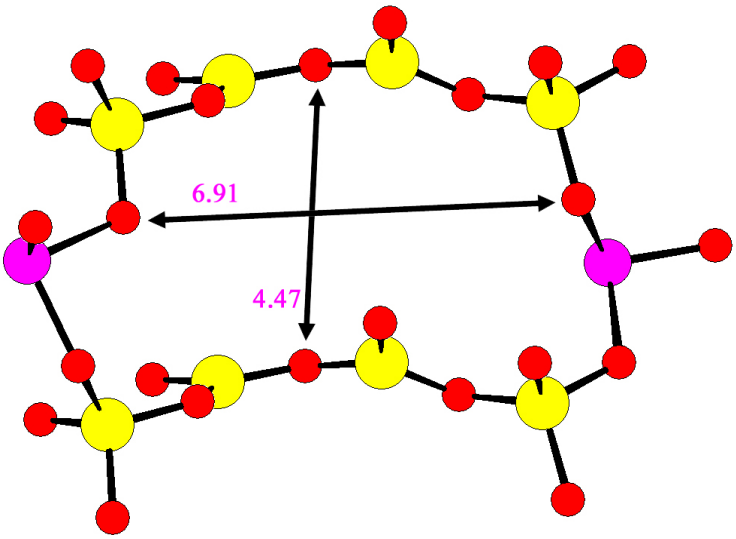
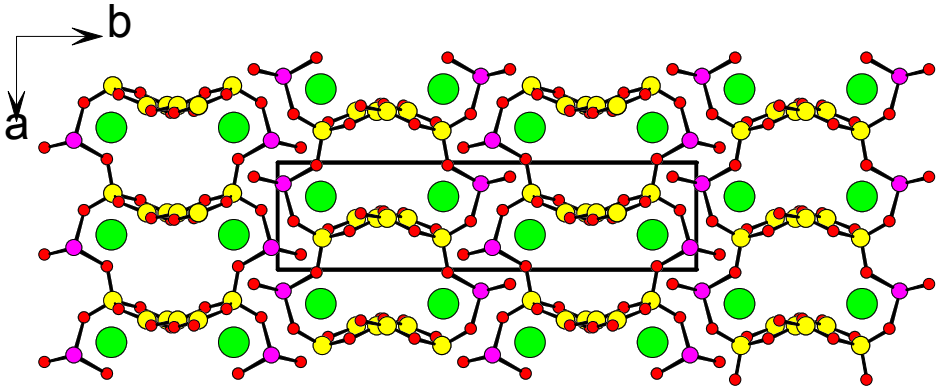


(a)



(b)



(c)

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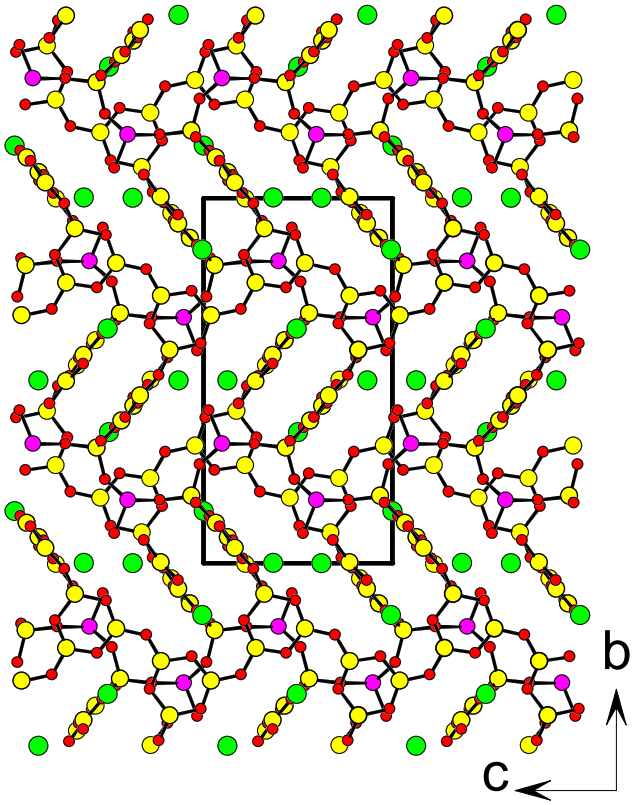
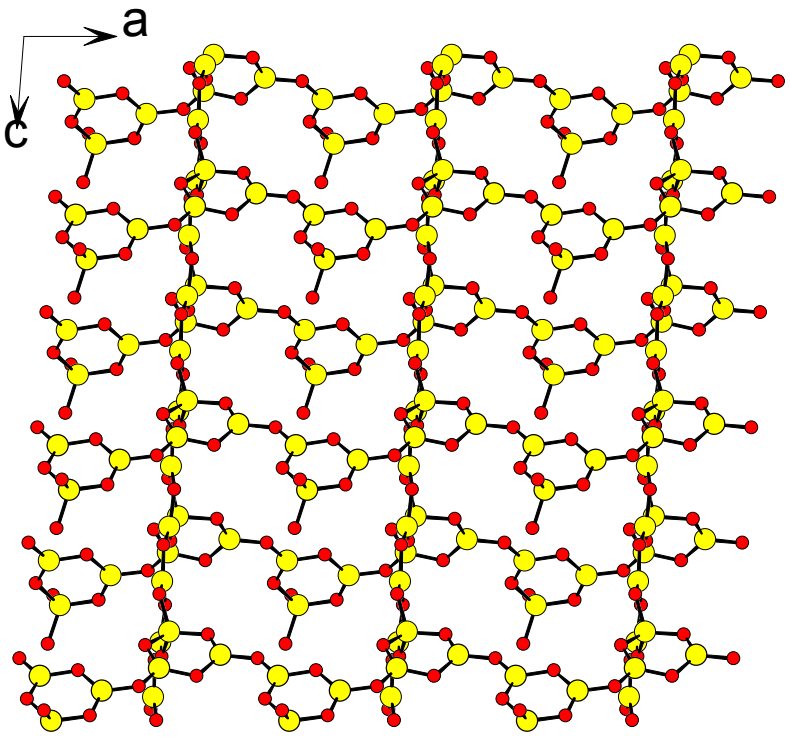
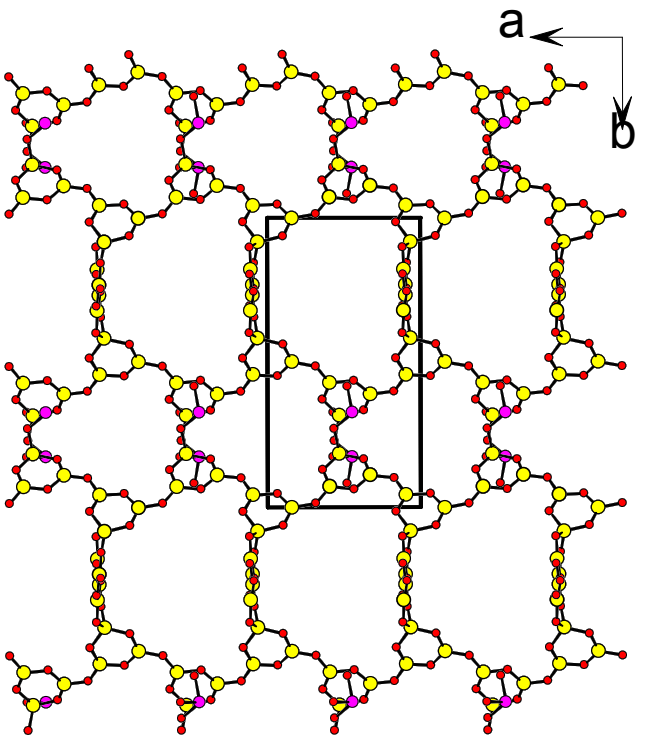


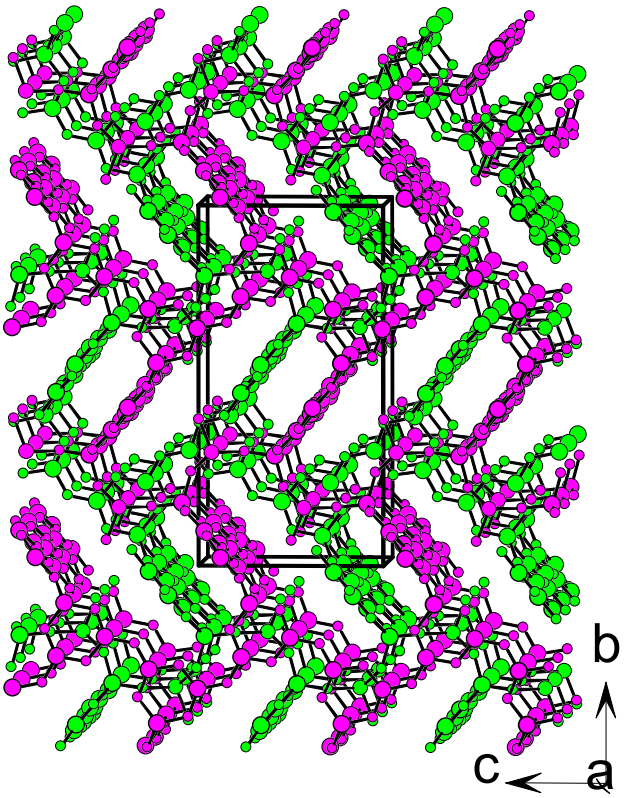
(a)



(b)



(c)



(d)

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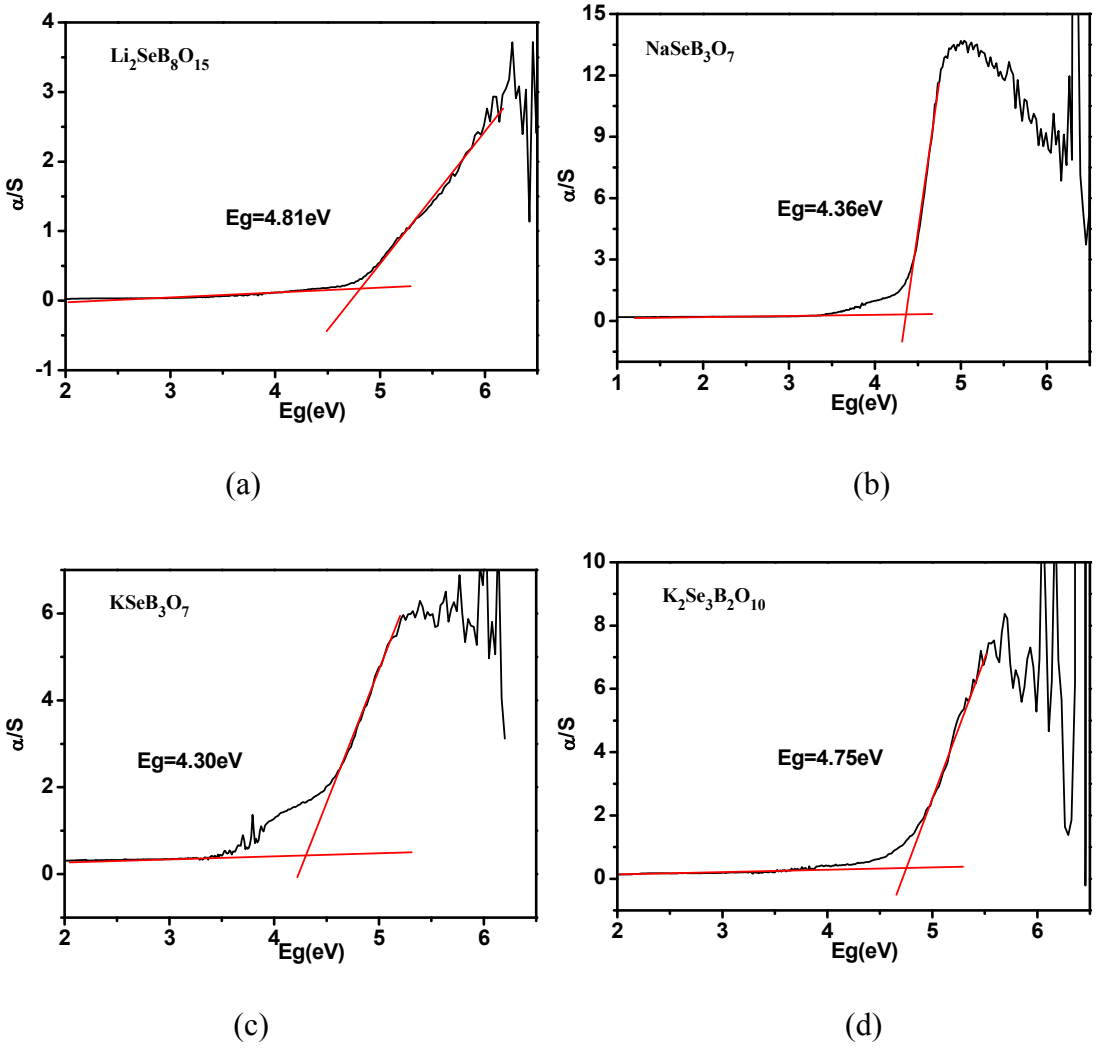

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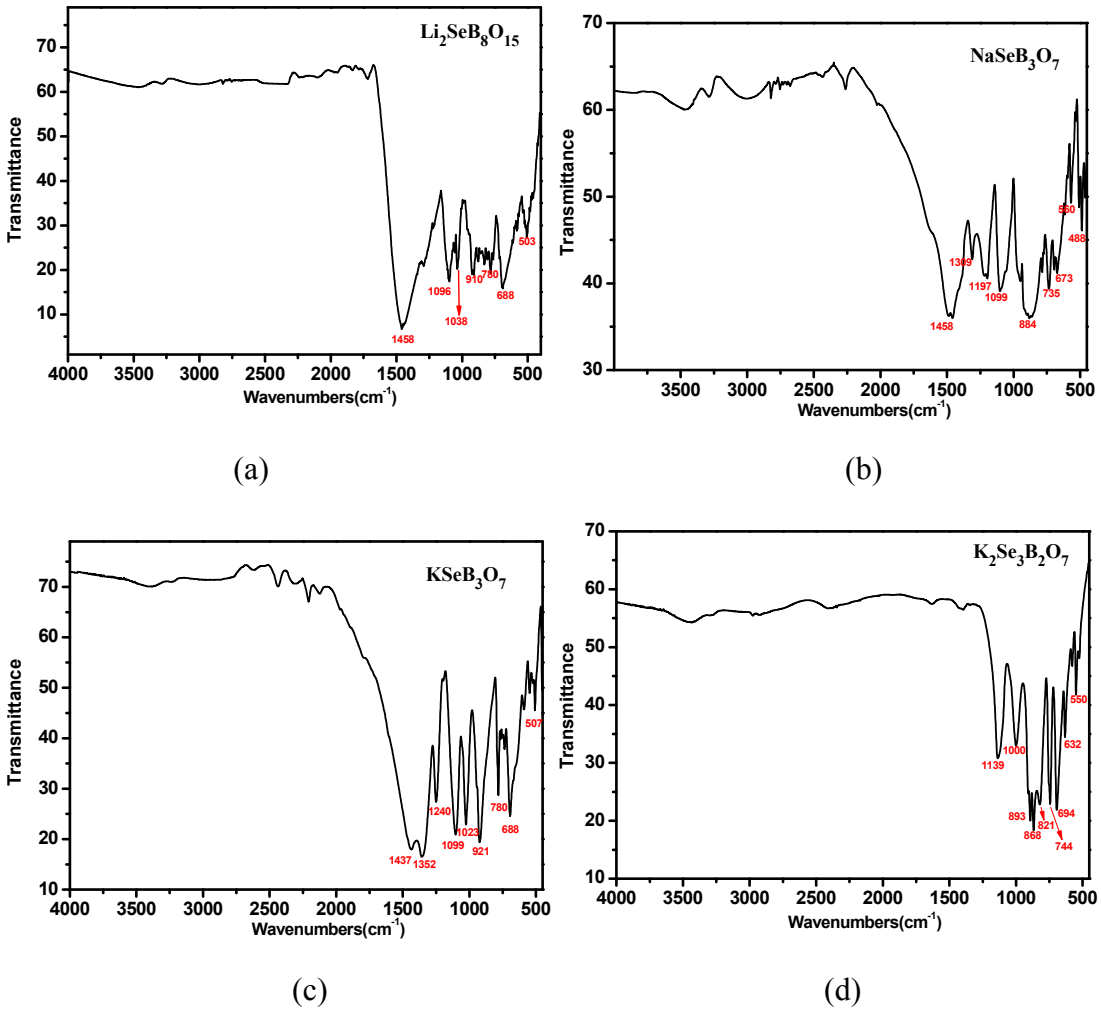

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