Supplementary Materials for

Stabilization of superionic-conducting high-temperature phase of $Li(CB_9H_{10})$ via solid solution formation with $Li_2(B_{12}H_{12})$

Sangryun Kim[1,★], Kazuaki Kisu[2], and Shin−ichi Orimo[1,2,★]

[1]Institute for Materials Research, Tohoku University, 2−1−1 Katahira, Aoba−ku, Sendai 980−8577, Japan

[2]WPI−Advanced Institute for Materials Research (WPI−AIMR), Tohoku University, 2−1−1 Katahira, Aoba−ku, Sendai 980−8577, Japan

[★]Corresponding authors. E−mail: sangryun@imr.tohoku.ac.jp, orimo@imr.tohoku.ac.jp

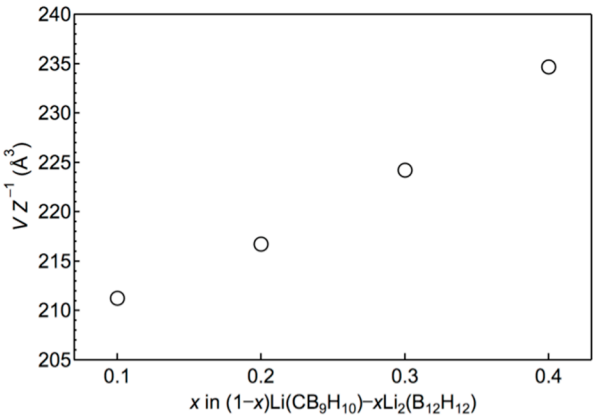

Figure S1. Compositional dependence of the lattice volume of the (1−x)Li(CB_9H_{10})−xLi$_2$($B_{12}H_{12}$) compounds with $0.1 \leq x \leq 0.4$. The compounds with $x = 0.1$ and 0.2 were indexed to a hexagonal unit cell consistent with that of the low-T phase (space group $P3c1$, ($Z = 6$)) [3] of Li(CB_9H_{10}) ($x = 0$). The $x = 0.3$ and 0.4 compounds were indexed to a hexagonal unit cell consistent with that of the high-T phase (space group $P31c$, ($Z = 2$)) [21] of Li(CB_9H_{10}) ($x = 0$).

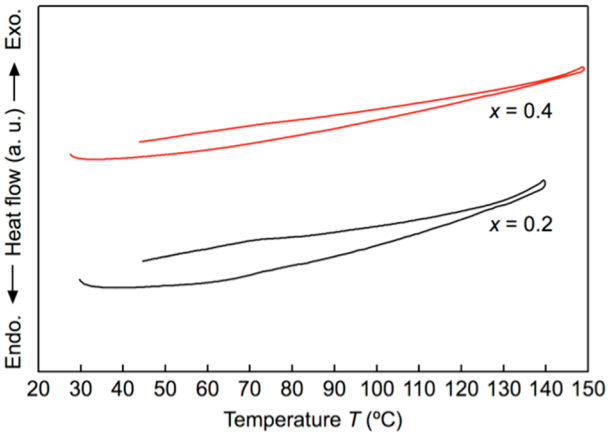

Figure S2. Enlarged DTA curves for the x = 0.2 and 0.4 compounds in Figure 2.

Table S1. Lithium-ion conductivities at 25 °C and activation energies of $(1-x)Li(CB_9H_{10})-xLi_2(B_{12}H_{12})$ ($0.1 \leq x \leq 0.5$).

x	Ionic Conductivity (S cm^{-1})	Activation Energy (kJ mol^{-1})
0.1	7.5×10^{-4}	–
0.2	1.4×10^{-3}	–
0.3	1.6×10^{-3}	40.5
0.4	1.7×10^{-3}	40.3
0.5	5.8×10^{-4}	–

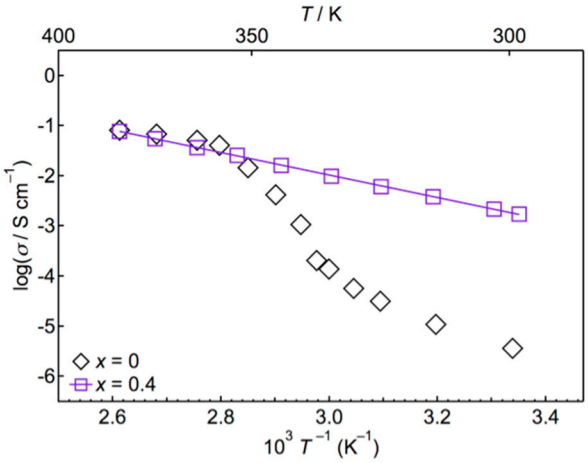

Figure S3. Arrhenius plots of the lithium-ion conductivities for the compounds with x = 0 ($Li(CB_9H_{10})$) and x = 0.4 ($0.6Li(CB_9H_{10})–0.4Li_2(B_{12}H_{12})$).

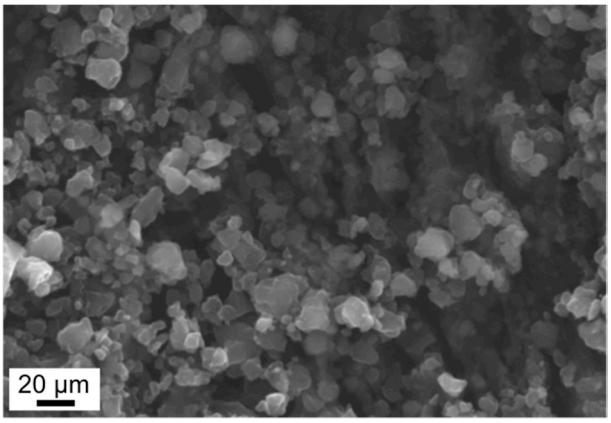

Figure S4. SEM micrograph of the x = 0.4 (0.6Li(CB_9H_{10})–0.4Li_2($B_{12}H_{12}$)) compound.

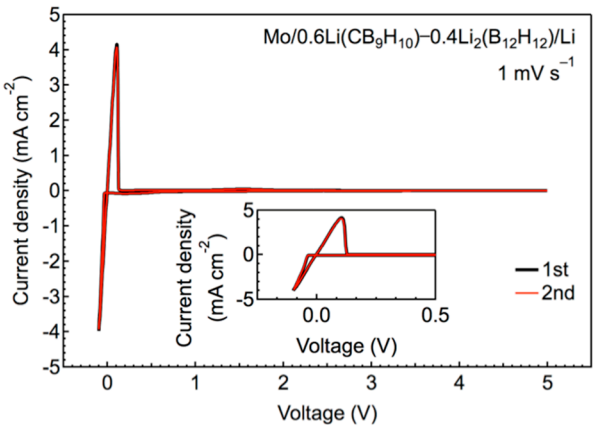

Figure S5. Cyclic voltammograms of a Mo/0.6Li(CB_9H_{10})–0.4Li_2($B_{12}H_{12}$)/Li cell at a scan rate of 1 mV s^{-1} during two cycles. Insets show the magnified plots in the low-voltage region.

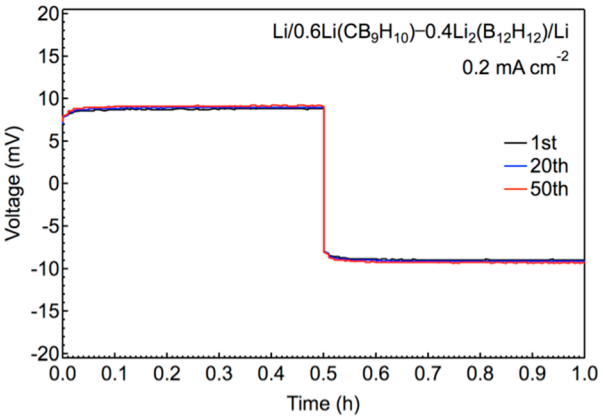

Figure S6. Galvanostatic cycling profiles of a Li/0.6Li(CB_9H_{10})–0.4Li_2($B_{12}H_{12}$)/Li cell at 0.2 mA cm^{-2}.

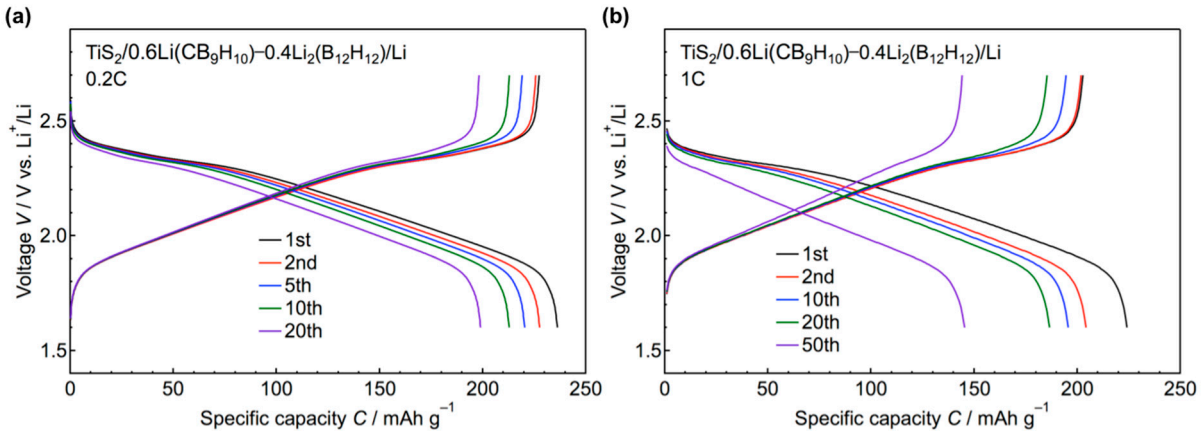

Figure S7. Discharge–charge profiles for the TiS_2/0.6Li(CB_9H_{10})–0.4Li_2($B_{12}H_{12}$)/Li cells for rates of (a) 0.2C and (b) 1C.