Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Role of ligands on the stability of B_nX_n and $CB_{n-1}X_n$ (n = 5–10; X = H, F, CN) and their potential as building blocks of electrolytes in lithium ion batteries

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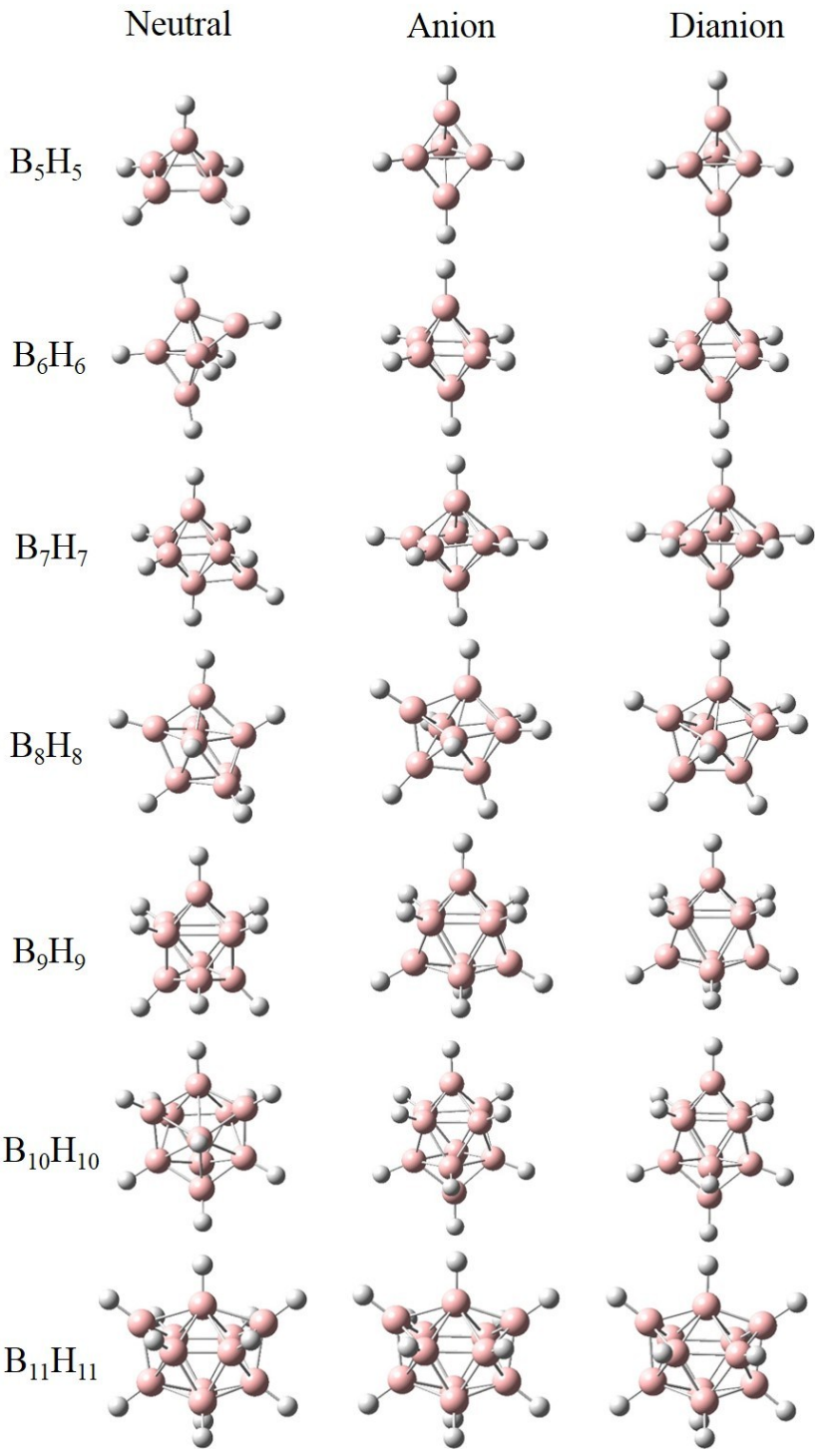

Fig. S1 The lowest energy structures of neutral, anion and dianion B_nH_n (n = 5–11).

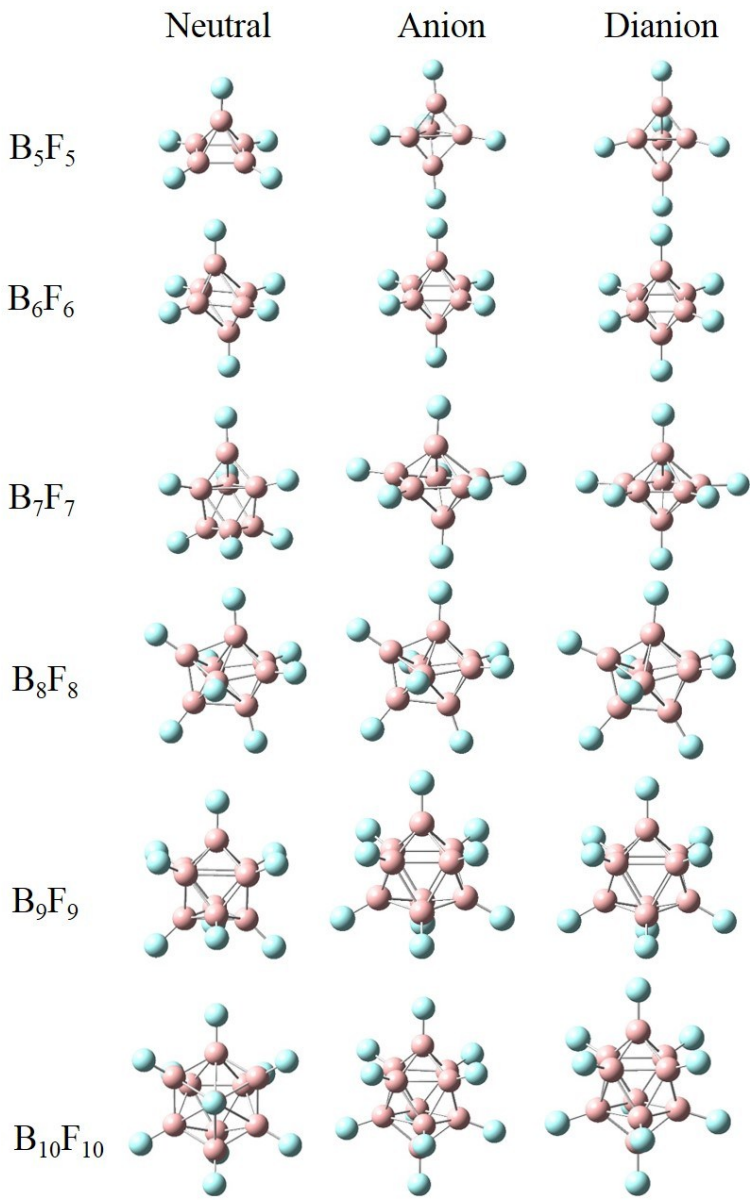

Fig. S2 The lowest energy structures of neutral, anion and dianion B_nF_n (n = 5–10).

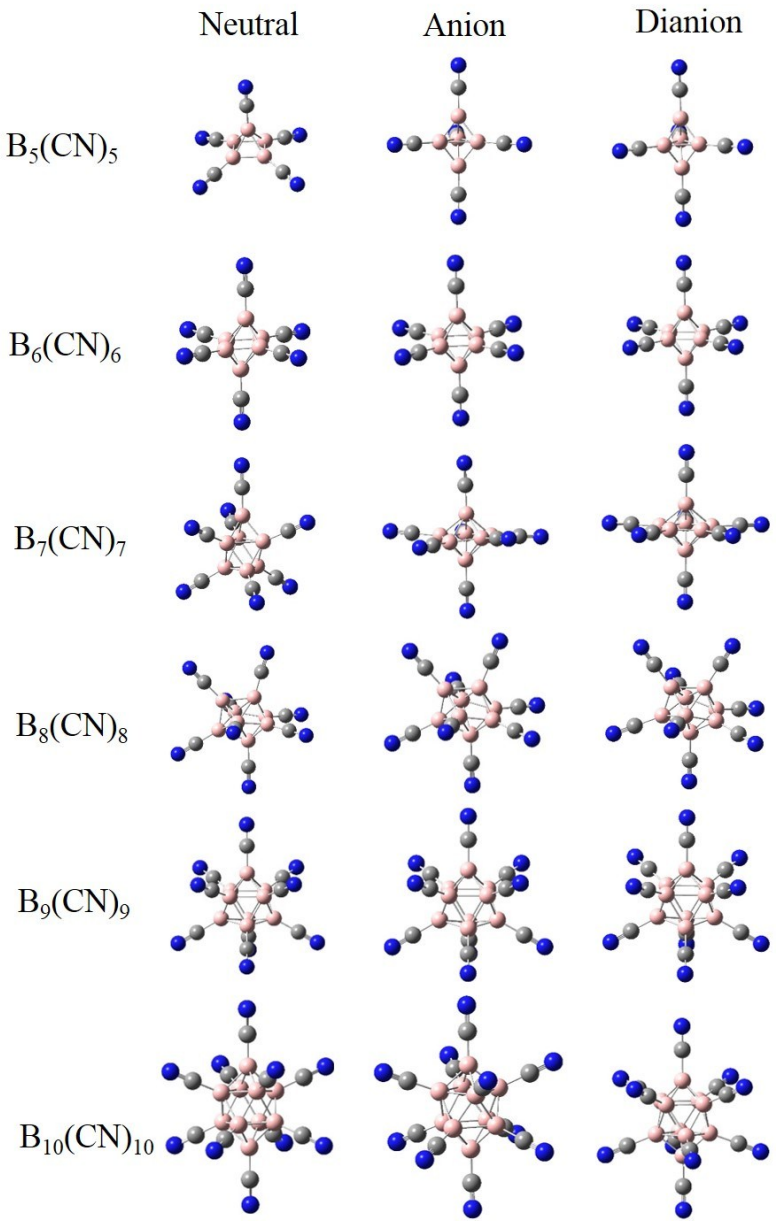

Fig. S3 The lowest energy structures of neutral, anion and dianion $B_n(CN)_n$ (n = 5–10).

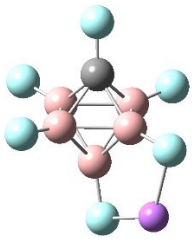

Fig. S4 The second lowest energy structure of $LiBC_5F_6$.