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

Supporting Information

Novel Benzimidazole Salts for Lithium Ion Battery Electrolytes: Effects of Substituents

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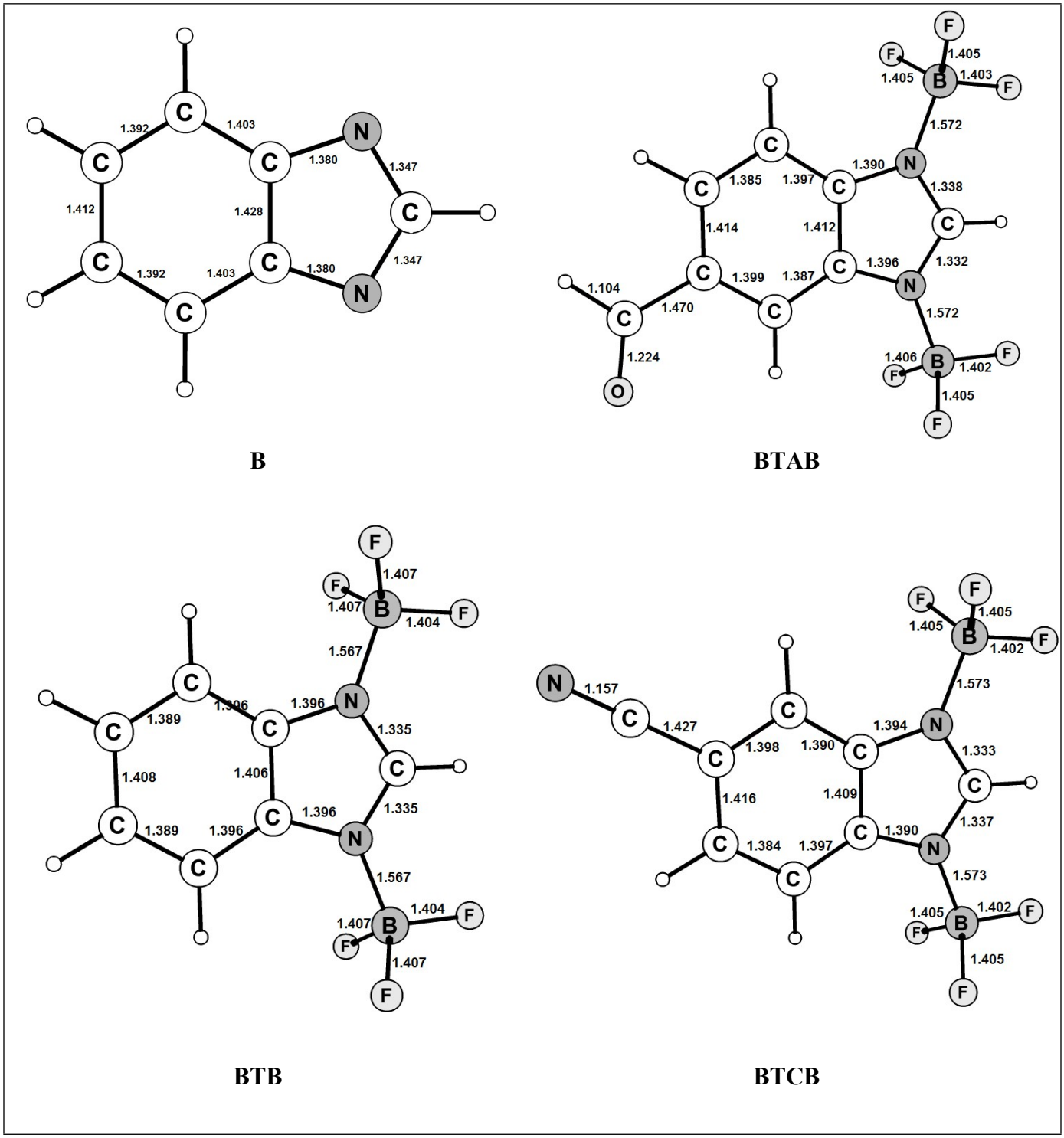
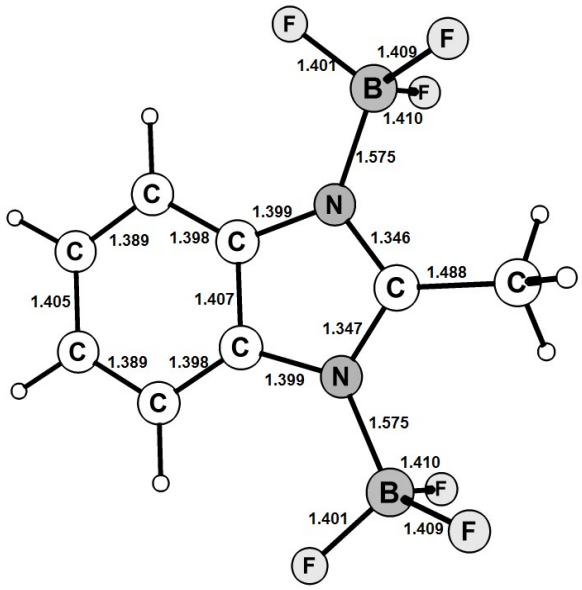
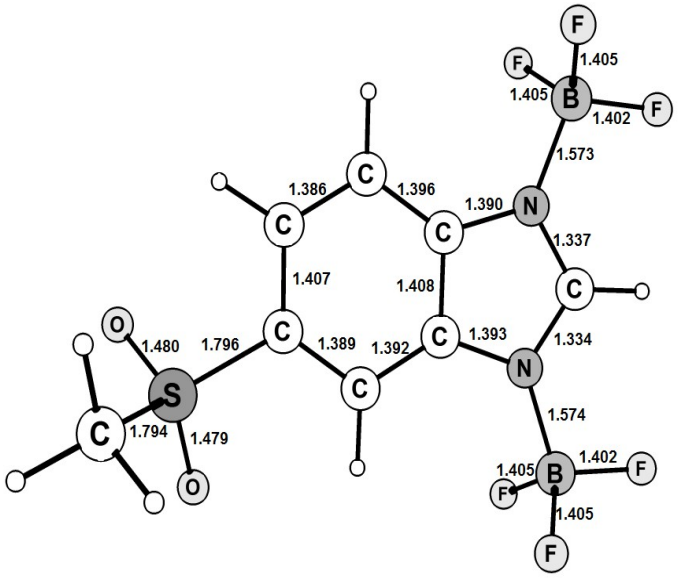
Figure S1. Optimized structures of the anions calculated with SMD-B3LYP/6-311++G(d,p). Values are given in Å.





BTMB



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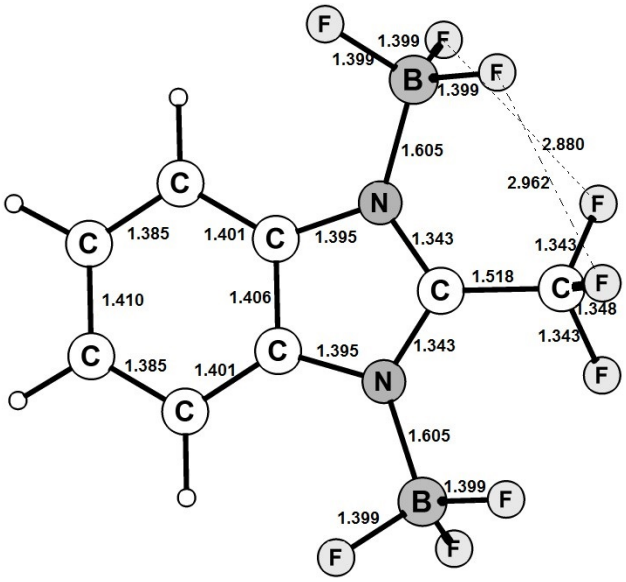

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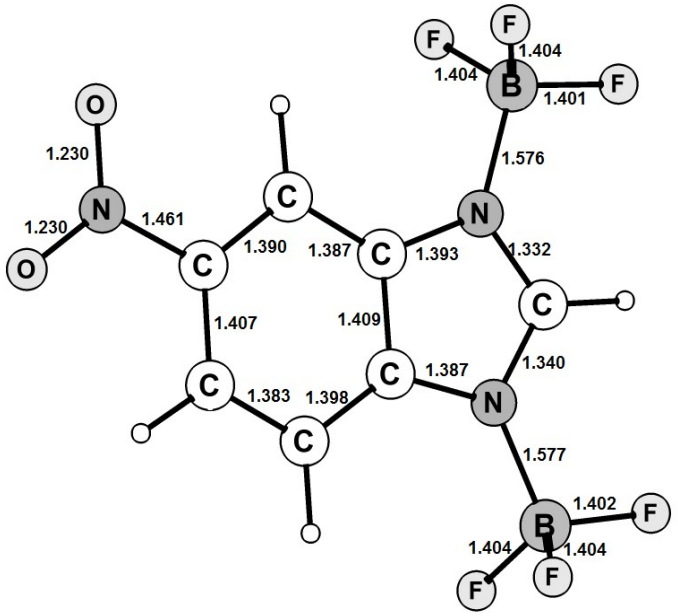

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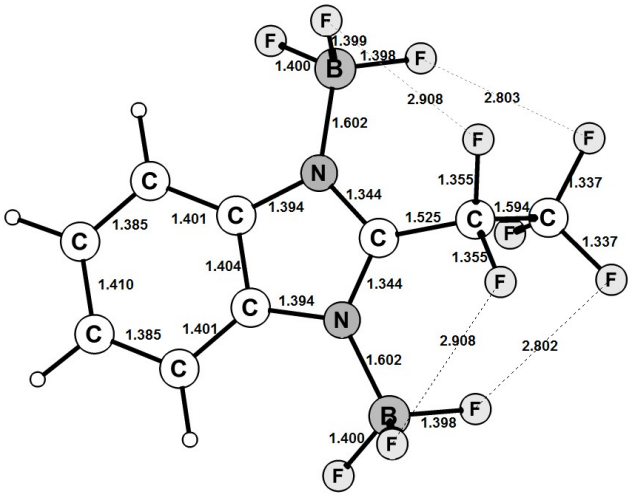

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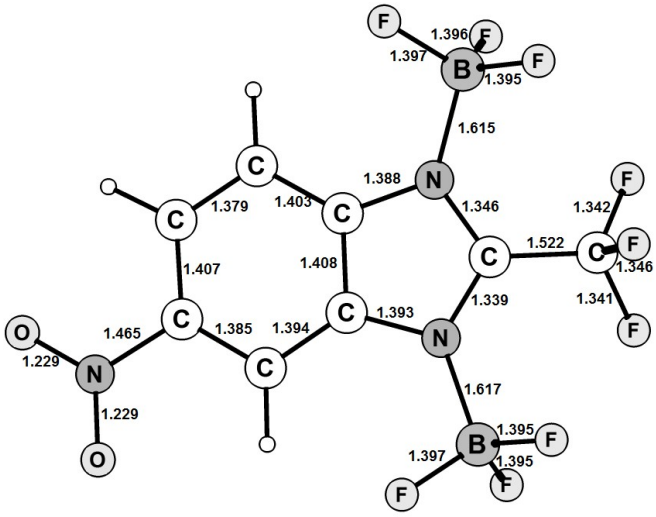

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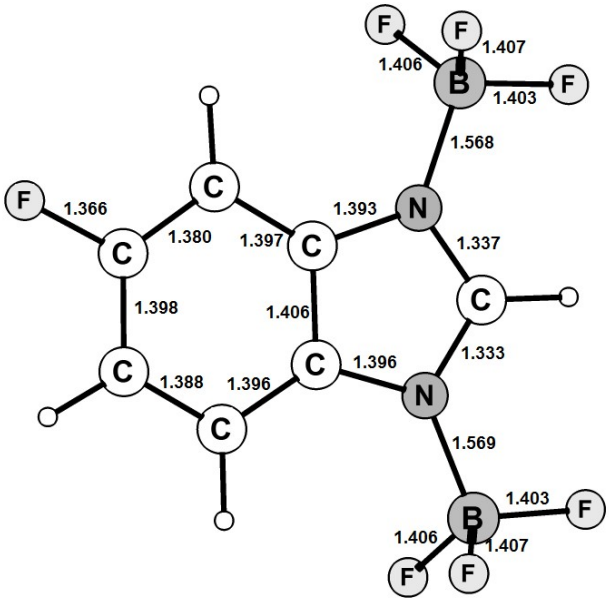
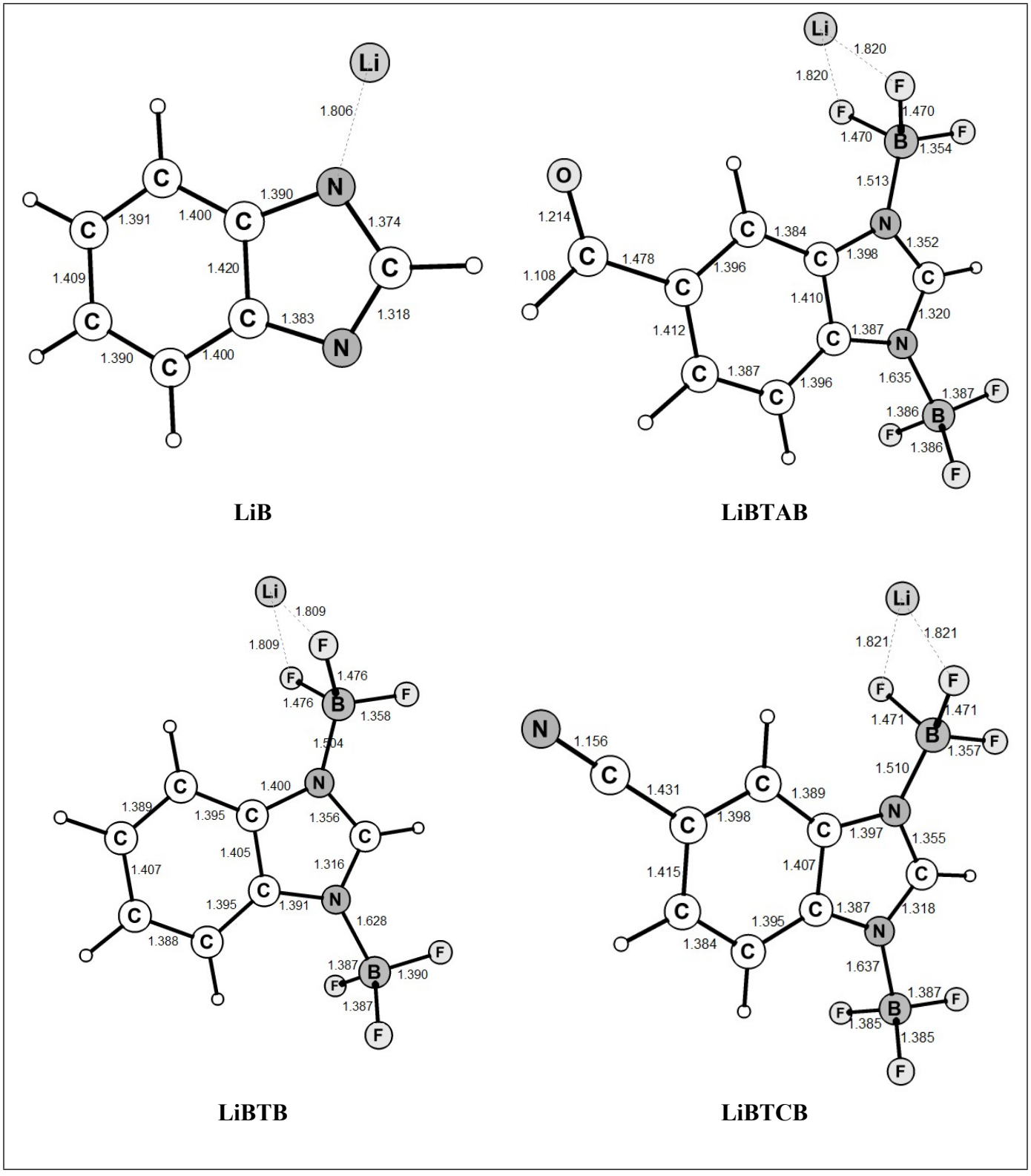
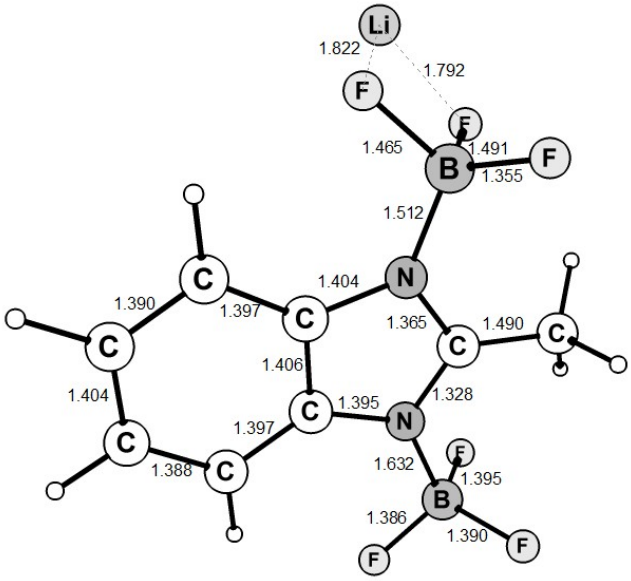


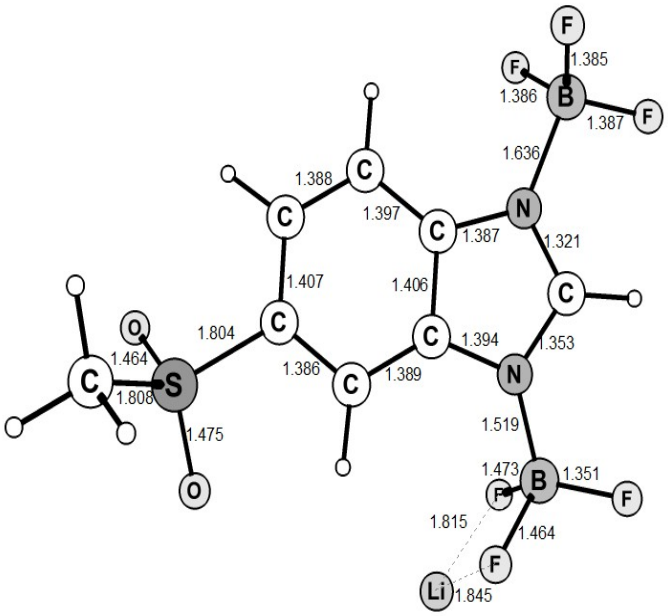
BTFB

Figure S2. Optimized structures of the ion pairs calculated with SMD-B3LYP/6-311++G(d,p). Values are given in Å.





LiBTMB



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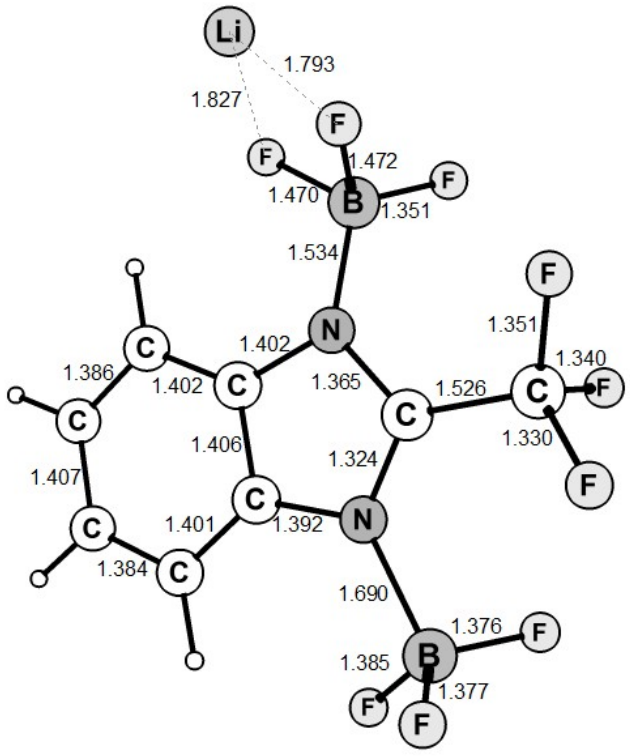

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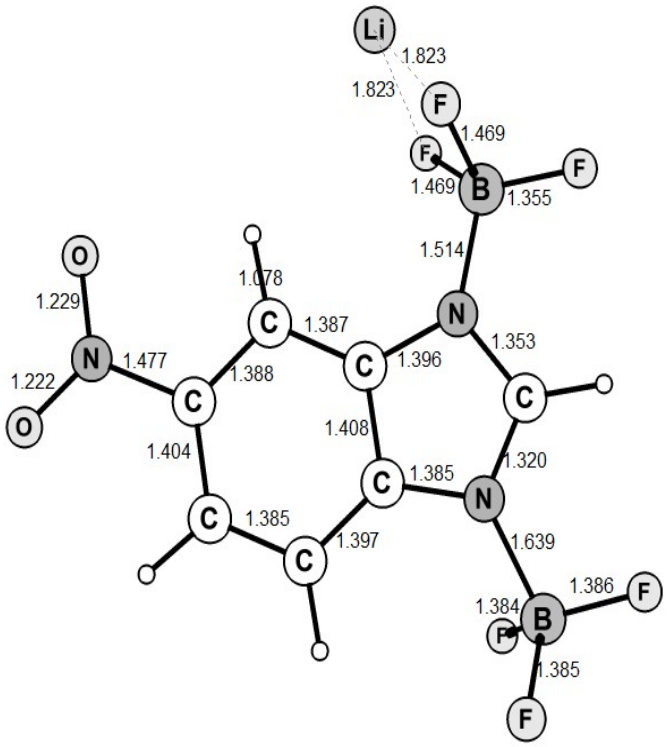

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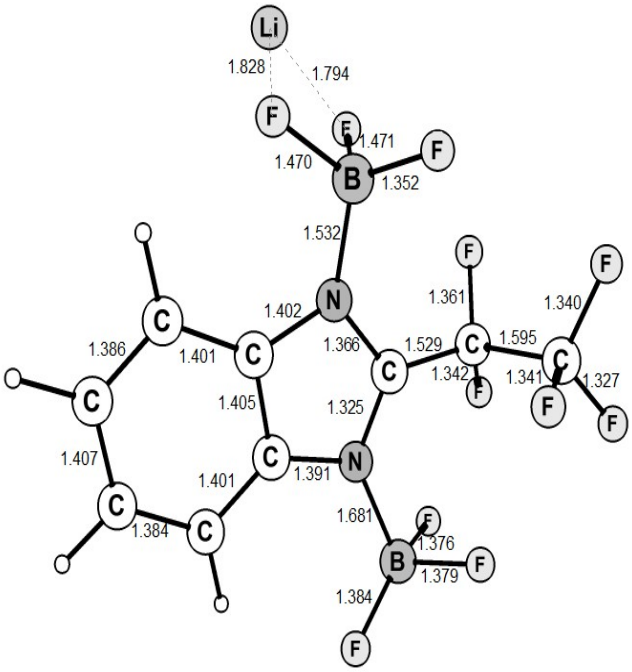

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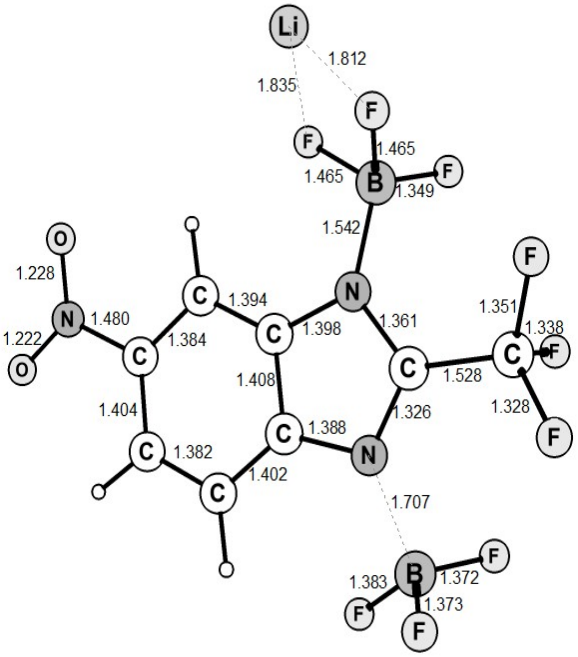

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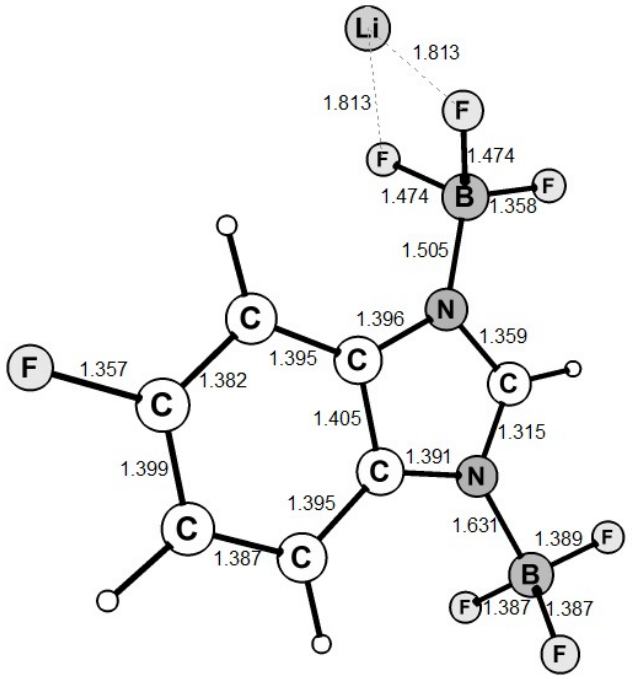

LiBTFB

Table S1. Lithium ion pair dissociation energies, ΔE_d (kcal /mol) in vacuum, implicit solvation and with BSSEs correction calculated at the level of B3LYP/6-311++G(d, p).

Structure	In vacuum	In implicit solvent	BSSE corrected
LiB	137.72	23.23	137.31
LiBTB	115.28	14.57	114.48
LiBTMB	116.29	14.98	115.48
LiBTTB	112.92	14.20	112.09
LiBTPB	112.50	14.02	111.67
LiBTFB	113.42	14.33	112.61
LiBTAB	114.14	14.38	113.34
LiBTCB	109.78	13.81	108.99
LiBTSB	112.67	14.03	111.85
LiBTNB	110.13	13.85	109.32
LiBTNTB	107.86	13.32	107.02
$LiPF_6$	133.95	15.12	132.64