

Supporting Information

Isomeric Thiophene-fused Benzocarborane Molecules — Different Lithium Doping Effect on the Nonlinear Optical Property

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Table S1. The β_{tot} value of Tb1-Li calculated by different methods with 6-31+G* basis set.

Tb1-Li	Mp2	CAM-B3LYP	BhandHLYP
β_x (au)	-1777	349	7
β_y (au)	-5505	-1188	-2799
β_z (au)	3739	1536	5557
β_{tot} (au)	6888	1973	6222

Table S2. The β_{tot} value of Tb1-Li is calculated by different basis set with BhandHLYP method.

Tb1-Li	6-31G*	6-31+G*	6-311+G*
β_x (au)	352	7	6
β_y (au)	-1227	-2799	-2571
β_z (au)	2825	5557	5110
β_{tot} (au)	3101	6222	5720