

SUPPORTING INFORMATION

Structures and Nonlinear Optical Properties of the Endohedral Metallofullerene-Superhalogen Compounds $\text{Li}@\text{C}_{60}\text{-BX}_4$ ($\text{X} = \text{F}, \text{Cl},$ Br)

Shu-Jian Wang^a, Ying Li^a, Yin-Feng Wang^b, Di Wu^{*a}, Zhi-Ru Li^a

^a *Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun 130023, People's Republic of China*

^b *Jiangxi Province Key Laboratory of Coordination Chemistry, Institute of Applied Chemistry, School of Chemistry and Chemical Engineering, Jinggangshan University, Ji'an, Jiangxi 343009, China*

Table S1. Optimized geometrical parameters of $\eta^6\text{-Li}@\text{C}_{60}\text{-BCl}_4$ at the B3LYP level with different basis sets.

$\eta^6\text{-Li}@\text{C}_{60}\text{-BCl}_4$	PG	d_{Li}	$\text{Li}\cdots\text{B}$	$d_{\text{X1}\cdots\text{C1}}$	$d_{\text{X1}\cdots\text{C2}}$	$d_{\text{X1}\cdots\text{C3}}$	$d_{\text{X2}\cdots\text{C3}}$	$d_{\text{X3}\cdots\text{C4}}$
Basis set A	C_s	1.525	5.620	3.651	3.690	3.722	3.100	3.100
Basis set B	C_s	1.553	5.583	3.643	3.684	3.718	3.097	3.097

Basis set A: 6-31G(d) for all the atoms. Basis set B: 6-31G(d) for the C, B, and Cl atoms, and 6-311+G(d) for trapped Li atom.

**Cartesian coordinate for the six endohedral
metallofullerene-superhalogen compounds Li@C₆₀-BX₄ (X=F, Cl, Br),
Li@C₆₀, and BX₄ (X=F, Cl, Br).**

η⁶-Li@C₆₀-BF₄ at B3LYP/6-31G* level

C	-1.24079200	0.71104500	3.03263400
C	-0.68855400	-0.55766900	3.48318500
C	0.69276300	-0.75538200	3.48142000
C	1.58044600	0.30564500	3.03157800
C	1.05171400	1.52399000	2.59973400
C	-0.38892600	1.73094400	2.60009400
C	-2.46973600	0.43369100	2.30667500
C	-2.67602100	-1.00562100	2.30619300
C	-1.57578400	-1.61775300	3.03374500
C	-1.04549900	-2.83399700	2.60041800
C	1.24537300	-2.02288300	3.03227300
C	2.68101900	-0.30598400	2.30678400
C	3.20550400	0.32431200	1.17629800
C	2.65673000	1.59357700	0.72812100
C	1.59911900	2.18240600	1.42370000
C	0.50145300	2.81583100	0.70144900
C	-0.73126100	2.52879000	1.42752500
C	-1.91888100	2.26390500	0.73046100
C	-2.79777000	1.18874800	1.17676600
C	-3.20248600	-1.63524100	1.17659700
C	-3.54231200	-0.85142700	0.00000000
C	-3.34594300	0.53164500	0.00000000
C	-2.79777000	1.18874800	-1.17676600
C	-1.91888100	2.26390500	-0.73046100
C	-0.73126100	2.52879000	-1.42752500
C	0.50145300	2.81583100	-0.70144900
C	1.59911900	2.18240600	-1.42370000
C	2.65673000	1.59357700	-0.72812100
C	2.47329200	-1.74476100	2.30535800
C	2.47329200	-1.74476100	-2.30535800
C	2.80043300	-2.49670600	-1.17614400
C	1.91341200	-3.55684000	-0.72684400
C	0.73474600	-3.82437900	-1.42467300
C	0.39352300	-3.04055100	-2.60016400
C	0.69276300	-0.75538200	-3.48142000
C	1.58044600	0.30564500	-3.03157800

C	2.68101900	-0.30598400	-2.30678400
C	3.20550400	0.32431200	-1.17629800
C	3.54699100	-0.45938200	0.00000000
C	3.34847100	-1.84087900	0.00000000
C	1.91341200	-3.55684000	0.72684400
C	0.73474600	-3.82437900	1.42467300
C	-0.49315700	-4.10169700	0.69772500
C	-0.49315700	-4.10169700	-0.69772500
C	-1.59370300	-3.48955500	-1.42424800
C	-1.04549900	-2.83399700	-2.60041800
C	-1.57578400	-1.61775300	-3.03374500
C	-0.68855400	-0.55766900	-3.48318500
C	1.05171400	1.52399000	-2.59973400
C	-0.38892600	1.73094400	-2.60009400
C	-1.24079200	0.71104500	-3.03263400
C	-2.46973600	0.43369100	-2.30667500
C	-2.67602100	-1.00562100	-2.30619300
C	-3.20248600	-1.63524100	-1.17659700
C	-2.65079100	-2.90302100	-0.72689800
C	-2.65079100	-2.90302100	0.72689800
C	-1.59370300	-3.48955500	1.42424800
C	2.80043300	-2.49670600	1.17614400
C	0.39352300	-3.04055100	2.60016400
C	1.24537300	-2.02288300	-3.03227300
F	0.70531800	5.25243400	1.14940500
F	-1.27581600	5.09046700	0.00000000
F	0.70531800	5.25243400	-1.14940500
Li	-0.31724700	0.84987200	0.00000000
B	-0.00100800	5.71145600	0.00000000
F	-0.10820300	7.08058400	0.00000000

η^5 -Li@C₆₀-BF₄ at B3LYP/6-31G* level

C	-0.00750700	1.19055800	3.03503900
C	-0.44961900	-0.11959500	3.48088200
C	0.44035000	-1.19658300	3.48272300
C	1.80836100	-1.00642300	3.03276700
C	2.23440200	0.25384700	2.60388800
C	1.30832700	1.37474800	2.60468900
C	-1.10346000	1.80989500	2.30184700
C	-2.22489000	0.88212600	2.30533900
C	-1.82010800	-0.30925800	3.03115300
C	-2.24369200	-1.56772900	2.60025500
C	-0.00233500	-2.50647700	3.03353000

C	2. 21384000	-2. 19832800	2. 30574600
C	3. 02810800	-2. 08657100	1. 17687100
C	3. 46977300	-0. 77622700	0. 72726800
C	3. 08239400	0. 37046200	1. 42754600
C	2. 68486500	1. 57192900	0. 70202900
C	1. 58410500	2. 19604300	1. 42941600
C	0. 53152300	2. 80846200	0. 73246600
C	-0. 84292400	2. 59074100	1. 17678000
C	-3. 03648000	0. 76954400	1. 17622800
C	-2. 76239000	1. 58046000	0. 00000000
C	-1. 68757800	2. 46849000	0. 00000000
C	-0. 84292400	2. 59074100	-1. 17678000
C	0. 53152300	2. 80846200	-0. 73246600
C	1. 58410500	2. 19604300	-1. 42941600
C	2. 68486500	1. 57192900	-0. 70202900
C	3. 08239400	0. 37046200	-1. 42754600
C	3. 46977300	-0. 77622700	-0. 72726800
C	1. 09364800	-3. 12563300	2. 30631400
C	1. 09364800	-3. 12563300	-2. 30631400
C	0. 83125600	-3. 90083100	-1. 17605700
C	-0. 53790000	-4. 09148300	-0. 72666900
C	-1. 59005800	-3. 49685200	-1. 42432500
C	-1. 31656800	-2. 68760300	-2. 60096300
C	0. 44035000	-1. 19658300	-3. 48272300
C	1. 80836100	-1. 00642300	-3. 03276700
C	2. 21384000	-2. 19832800	-2. 30574600
C	3. 02810800	-2. 08657100	-1. 17687100
C	2. 75485100	-2. 89582700	0. 00000000
C	1. 67800700	-3. 78340200	0. 00000000
C	-0. 53790000	-4. 09148300	0. 72666900
C	-1. 59005800	-3. 49685200	1. 42432500
C	-2. 68619800	-2. 87762800	0. 69780600
C	-2. 68619800	-2. 87762800	-0. 69780600
C	-3. 08987800	-1. 68549800	-1. 42495400
C	-2. 24369200	-1. 56772900	-2. 60025500
C	-1. 82010800	-0. 30925800	-3. 03115300
C	-0. 44961900	-0. 11959500	-3. 48088200
C	2. 23440200	0. 25384700	-2. 60388800
C	1. 30832700	1. 37474800	-2. 60468900
C	-0. 00750700	1. 19055800	-3. 03503900
C	-1. 10346000	1. 80989500	-2. 30184700
C	-2. 22489000	0. 88212600	-2. 30533900
C	-3. 03648000	0. 76954400	-1. 17622800
C	-3. 47743700	-0. 54001300	-0. 72701400

C	-3.47743700	-0.54001300	0.72701400
C	-3.08987800	-1.68549800	1.42495400
C	0.83125600	-3.90083100	1.17605700
C	-1.31656800	-2.68760300	2.60096300
C	-0.00233500	-2.50647700	-3.03353000
F	0.64326000	5.21836000	1.14704300
F	-1.34539000	5.24725700	0.00000000
F	0.64326000	5.21836000	-1.14704300
Li	0.69785000	0.69956300	0.00000000
B	-0.02282900	5.74528500	0.00000000
F	0.00781500	7.11703400	0.00000000

η^6 -Li@C₆₀-BCl₄ at B3LYP/6-31G* level

C	-1.28038100	0.13549400	3.03287400
C	-0.69055300	-1.11589200	3.48341600
C	0.69622600	-1.27225300	3.48170500
C	1.55224400	-0.18555100	3.03262200
C	0.98722100	1.01740800	2.60137500
C	-0.45867700	1.18091500	2.60252700
C	-2.50072600	-0.17870800	2.30659300
C	-2.66385700	-1.62342100	2.30661000
C	-1.54575400	-2.20213700	3.03415600
C	-0.97933000	-3.40174700	2.60076700
C	1.28651300	-2.52286900	3.03282900
C	2.67017500	-0.76379300	2.30796400
C	3.17530900	-0.11803800	1.17697500
C	2.58739600	1.13254800	0.72904200
C	1.51535100	1.69031500	1.42600600
C	0.39793100	2.29114400	0.70196500
C	-0.82544900	1.96505100	1.42815100
C	-2.00470500	1.66419200	0.73041800
C	-2.85402200	0.56604900	1.17744700
C	-3.17080300	-2.26820700	1.17663600
C	-3.53479100	-1.49524000	0.00000000
C	-3.38180100	-0.10671200	0.00000000
C	-2.85402200	0.56604900	-1.17744700
C	-2.00470500	1.66419200	-0.73041800
C	-0.82544900	1.96505100	-1.42815100
C	0.39793100	2.29114400	-0.70196500
C	1.51535100	1.69031500	-1.42600600
C	2.58739600	1.13254800	-0.72904200
C	2.50559800	-2.20812000	2.30612900
C	2.50559800	-2.20812000	-2.30612900

C	2.85424800	-2.94928900	-1.17626200
C	1.99987800	-4.03558500	-0.72689100
C	0.82968500	-4.33837700	-1.42487300
C	0.46538500	-3.56524500	-2.60055000
C	0.69622600	-1.27225300	-3.48170500
C	1.55224400	-0.18555100	-3.03262200
C	2.67017500	-0.76379300	-2.30796400
C	3.17530900	-0.11803800	-1.17697500
C	3.53960900	-0.89070700	0.00000000
C	3.38230000	-2.27715100	0.00000000
C	1.99987800	-4.03558500	0.72689100
C	0.82968500	-4.33837700	1.42487300
C	-0.38906600	-4.65213900	0.69778300
C	-0.38906600	-4.65213900	-0.69778300
C	-1.50752200	-4.07330400	-1.42424000
C	-0.97933000	-3.40174700	-2.60076700
C	-1.54575400	-2.20213700	-3.03415600
C	-0.69055300	-1.11589200	-3.48341600
C	0.98722100	1.01740800	-2.60137500
C	-0.45867700	1.18091500	-2.60252700
C	-1.28038100	0.13549400	-3.03287400
C	-2.50072600	-0.17870800	-2.30659300
C	-2.66385700	-1.62342100	-2.30661000
C	-3.17080300	-2.26820700	-1.17663600
C	-2.58161100	-3.51867600	-0.72690600
C	-2.58161100	-3.51867600	0.72690600
C	-1.50752200	-4.07330400	1.42424000
C	2.85424800	-2.94928900	1.17626200
C	0.46538500	-3.56524500	2.60055000
C	1.28651300	-2.52286900	-3.03282900
Li	-0.36603500	0.28696200	0.00000000
B	-0.00590500	5.89514200	0.00000000
Cl	0.88994300	5.23583100	1.53830000
Cl	-1.77144700	5.23326200	0.00000000
Cl	0.00610600	7.73537500	0.00000000
Cl	0.88994300	5.23583100	-1.53830000

η^5 -Li@C₆₀-BCl₄ at B3LYP/6-31G* level

C	-0.40729400	-1.76364100	3.48280100
C	0.10989600	-3.04615600	3.03403700
C	1.43196400	-3.14989500	2.60022700
C	2.29332400	-1.97889000	2.60018700
C	1.79882600	-0.74719300	3.03235100

C	0.41946800	-0.63761000	3.48166900
C	-1.78459400	-1.65287700	3.03317300
C	-2.12004100	-2.86591300	2.30577200
C	-0.94849000	-3.72726100	2.30663100
C	-0.64177700	-4.48541500	1.17608700
C	1.75201500	-3.94251000	1.42409400
C	3.14485300	-2.04753600	1.42459500
C	3.46664500	-0.88203400	0.72703700
C	2.95048300	0.40024400	1.17611800
C	2.13478700	0.46601300	2.30686700
C	0.96180100	1.32632800	2.30350900
C	-0.09797600	0.64434700	3.03374900
C	-1.42386400	0.75317700	2.60723500
C	-2.28380500	-0.41950800	2.60559300
C	-2.93960800	-2.80173900	1.17692400
C	-3.45596500	-1.51909500	0.72772800
C	-3.13689500	-0.35222400	1.42888800
C	-2.80967300	0.87006300	0.70258200
C	-1.74652700	1.55468700	1.43050900
C	-0.72720100	2.22114100	0.73147300
C	0.65646300	2.08855000	1.17627600
C	1.50805800	2.02185600	0.00000000
C	2.63176200	1.19358800	0.00000000
C	2.81096900	-3.26124200	0.69782700
C	1.79882600	-0.74719300	-3.03235100
C	2.29332400	-1.97889000	-2.60018700
C	1.43196400	-3.14989500	-2.60022700
C	0.10989600	-3.04615600	-3.03403700
C	-0.40729400	-1.76364100	-3.48280100
C	-0.09797600	0.64434700	-3.03374900
C	0.96180100	1.32632800	-2.30350900
C	2.13478700	0.46601300	-2.30686700
C	2.95048300	0.40024400	-1.17611800
C	3.46664500	-0.88203400	-0.72703700
C	3.14485300	-2.04753600	-1.42459500
C	1.75201500	-3.94251000	-1.42409400
C	0.73605300	-4.59729200	-0.72666100
C	-0.64177700	-4.48541500	-1.17608700
C	-0.94849000	-3.72726100	-2.30663100
C	-2.12004100	-2.86591300	-2.30577200
C	-1.78459400	-1.65287700	-3.03317300
C	-2.28380500	-0.41950800	-2.60559300
C	-1.42386400	0.75317700	-2.60723500
C	0.65646300	2.08855000	-1.17627600

C	-0.72720100	2.22114100	-0.73147300
C	-1.74652700	1.55468700	-1.43050900
C	-2.80967300	0.87006300	-0.70258200
C	-3.13689500	-0.35222400	-1.42888800
C	-3.45596500	-1.51909500	-0.72772800
C	-2.93960800	-2.80173900	-1.17692400
C	-2.62067000	-3.59389500	0.00000000
C	-1.49356600	-4.41680600	0.00000000
C	2.81096900	-3.26124200	-0.69782700
C	0.73605300	-4.59729200	0.72666100
C	0.41946800	-0.63761000	-3.48166900
Li	-0.79342000	0.09091300	0.00000000
B	0.01310200	5.93935000	0.00000000
Cl	-0.86306100	5.25358300	1.53614200
Cl	-0.86306100	5.25358300	-1.53614200
Cl	-0.04657300	7.77870800	0.00000000
Cl	1.79829800	5.32847100	0.00000000

η^6 -Li@C₆₀-BBr₄ at B3LYP/6-31G(d) level

C	0.64969700	3.01096400	1.29233100
C	1.92158400	3.47020900	0.75531900
C	2.12757500	3.49511500	-0.62476700
C	1.07184100	3.06422000	-1.52824900
C	-0.15029400	2.62205500	-1.01347600
C	-0.36533800	2.59540200	0.42487000
C	0.91883200	2.26193600	2.50821000
C	2.35669600	2.25471100	2.72241800
C	2.97612300	3.00224100	1.63989300
C	4.19428300	2.57700100	1.10771700
C	3.39763100	3.05525200	-1.17875100
C	1.68804600	2.36127400	-2.63846800
C	1.05839600	1.24000600	-3.18634000
C	-0.21267500	0.78416300	-2.65383200
C	-0.80720300	1.45969300	-1.58775200
C	-1.45827200	0.71800200	-0.50840400
C	-1.16478600	1.41843800	0.74019200
C	-0.90432900	0.69791100	1.91387900
C	0.16044300	1.12599300	2.81022900
C	2.98151000	1.11334100	3.22917900
C	2.19428400	-0.06874900	3.54184600
C	0.81285300	-0.06320300	3.33801300
C	0.15767300	-1.22963600	2.76472300
C	-0.90582300	-0.76453700	1.88551800

C	-1.16792700	-1.43835400	0.68483500
C	-1.45934500	-0.68933300	-0.53568300
C	-0.81032700	-1.39031400	-1.64283900
C	-0.21452600	-0.67554300	-2.68233500
C	3.12533000	2.35309500	-2.42245300
C	3.11983600	-2.26006500	-2.51171800
C	3.87430000	-1.12471900	-2.81175600
C	4.92972700	-0.69362200	-1.91091000
C	5.18992900	-1.41429000	-0.74424000
C	4.40341900	-2.59558900	-0.43049700
C	2.11931500	-3.46855700	-0.75957400
C	1.06464700	-3.00058800	-1.64564100
C	1.68253700	-2.25658300	-2.72788100
C	1.05554500	-1.11352400	-3.23193000
C	1.84215200	0.06880300	-3.54520600
C	3.22204300	0.06320100	-3.33905900
C	4.93133000	0.76017300	-1.88271000
C	5.19332900	1.43451000	-0.68909400
C	5.46264700	0.68365700	0.52583000
C	5.46093400	-0.71165900	0.49883300
C	4.84148500	-1.45857600	1.58130100
C	4.18819400	-2.62322100	1.00708500
C	2.96892700	-3.06563500	1.52241600
C	1.91330300	-3.49656500	0.62044500
C	-0.15643600	-2.57574300	-1.11403400
C	-0.37154000	-2.60431200	0.32416800
C	0.64247000	-3.05558800	1.17488200
C	0.91336500	-2.35481200	2.41883400
C	2.35118400	-2.35924000	2.63312600
C	2.97865800	-1.23975500	3.18364400
C	4.24948800	-0.78122700	2.64824700
C	4.25126900	0.67276900	2.67643800
C	4.84482400	1.38952600	1.63639500
C	3.87700000	1.22834500	-2.76615600
C	4.40959800	2.60460800	-0.32978600
C	3.39039100	-3.01047100	-1.29617500
Li	0.50260100	-0.00308800	0.26742600
B	-5.05569400	-0.00072600	0.01887300
Br	-4.37077300	-0.04570100	1.93184200
Br	-4.32366600	1.68159100	-0.90774700
Br	-7.04620500	0.00246900	-0.04213600
Br	-4.32576400	-1.63843700	-0.98548100

η^5 -Li@C₆₀-BBr₄ at B3LYP/6-31G(d) level

C	1. 78437900	0. 69948200	1. 42930800
C	1. 45076000	-0. 09734800	2. 60561500
C	0. 12390500	-0. 18782400	3. 03339800
C	-0. 92601700	0. 50779900	2. 30145800
C	-0. 61008900	1. 26819700	1. 17625700
C	0. 77677300	1. 39190400	0. 73360900
C	2. 83539100	-0. 00053000	0. 70257200
C	3. 14765700	-1. 22623200	1. 42842400
C	2. 29442200	-1. 28152700	2. 60500900
C	1. 77840200	-2. 50796400	3. 03317100
C	-0. 41123700	-1. 46192900	3. 48133200
C	-2. 11162800	-0. 33522700	2. 30693500
C	-2. 92727000	-0. 39014200	1. 17532200
C	-2. 59792000	0. 39801500	0. 00000000
C	-1. 46434300	1. 21583600	0. 00000000
C	-0. 61008900	1. 26819700	-1. 17625700
C	0. 77677300	1. 39190400	-0. 73360900
C	1. 78437900	0. 69948200	-1. 42930800
C	2. 83539100	-0. 00053000	-0. 70257200
C	3. 45204500	-2. 39723500	0. 72780000
C	3. 45204500	-2. 39723500	-0. 72780000
C	3. 14765700	-1. 22623200	-1. 42842400
C	2. 29442200	-1. 28152700	-2. 60500900
C	1. 45076000	-0. 09734800	-2. 60561500
C	0. 12390500	-0. 18782400	-3. 03339800
C	-0. 92601700	0. 50779900	-2. 30145800
C	-2. 11162800	-0. 33522700	-2. 30693500
C	-2. 92727000	-0. 39014200	-1. 17532200
C	-1. 79211200	-1. 55240200	3. 03169000
C	-2. 83917900	-4. 05293200	-0. 69796500
C	-2. 83917900	-4. 05293200	0. 69796500
C	-1. 78955200	-4. 74825400	1. 42421400
C	-0. 78254400	-5. 41663600	0. 72663200
C	-0. 78254400	-5. 41663600	-0. 72663200
C	-1. 45867300	-3. 96011400	-2. 60047600
C	-2. 30397900	-2. 77791200	-2. 60050700
C	-3. 15610800	-2. 83486300	-1. 42475600
C	-3. 46168300	-1. 66497200	-0. 72697900
C	-3. 46168300	-1. 66497200	0. 72697900
C	-3. 15610800	-2. 83486300	1. 42475600
C	-1. 45867300	-3. 96011400	2. 60047600
C	-0. 13515000	-3. 87483200	3. 03457400
C	0. 91379200	-4. 57008600	2. 30666100
C	0. 59669700	-5. 32386900	1. 17612600

C	1.44920900	-5.26667600	0.00000000
C	0.59669700	-5.32386900	-1.17612600
C	0.91379200	-4.57008600	-2.30666100
C	-0.13515000	-3.87483200	-3.03457400
C	-1.79211200	-1.55240200	-3.03169000
C	-0.41123700	-1.46192900	-3.48133200
C	0.39972400	-2.59973500	-3.48272400
C	1.77840200	-2.50796400	-3.03317100
C	2.09722300	-3.72514000	-2.30612400
C	2.91750600	-3.67186300	-1.17691500
C	2.58757400	-4.45947100	0.00000000
C	2.91750600	-3.67186300	1.17691500
C	2.09722300	-3.72514000	2.30612400
C	-2.30397900	-2.77791200	2.60050700
C	0.39972400	-2.59973500	3.48272400
C	-1.78955200	-4.74825400	-1.42421400
Li	0.75722100	-0.70560900	0.00000000
B	-0.01093700	5.09094700	0.00000000
Br	0.94829000	4.35785700	-1.65573500
Br	0.94829000	4.35785700	1.65573500
Br	0.02214700	7.08187200	0.00000000
Br	-1.93088700	4.39790300	0.00000000

Li@C₆₀ at B3LYP/6-31G* level

C	-1.28711300	-0.76357000	3.04093000
C	-0.69122000	-2.01201000	3.49359500
C	0.69566100	-2.16543200	3.49167400
C	1.55180900	-1.07889400	3.04111300
C	0.97831300	0.12460700	2.61308300
C	-0.46221000	0.28509300	2.61595300
C	-2.50896000	-1.07934600	2.32406400
C	-2.66689600	-2.51569300	2.31887100
C	-1.54626700	-3.09737800	3.04148800
C	-0.97523600	-4.29288000	2.60459900
C	1.29013700	-3.41337200	3.04040000
C	2.67029500	-1.65406600	2.32115000
C	3.17314500	-1.00030600	1.18139200
C	2.57795100	0.23633800	0.73278300
C	1.50118600	0.80162200	1.43033500
C	0.39046900	1.40869500	0.71513700
C	-0.82610500	1.07053400	1.43377000
C	-2.01065400	0.75568000	0.73621300
C	-2.85865300	-0.32779100	1.18262300
C	-3.16938100	-3.16636900	1.18057100

C	-3.52218300	-2.39250200	0.00000000
C	-3.37232600	-1.00387500	0.00000000
C	-2.85865300	-0.32779100	-1.18262300
C	-2.01065400	0.75568000	-0.73621300
C	-0.82610500	1.07053400	-1.43377000
C	0.39046900	1.40869500	-0.71513700
C	1.50118600	0.80162200	-1.43033500
C	2.57795100	0.23633800	-0.73278300
C	2.50916200	-3.09247500	2.31651800
C	2.50916200	-3.09247500	-2.31651800
C	2.85457300	-3.83545200	-1.17939100
C	2.00269400	-4.91621100	-0.72903000
C	0.82998100	-5.22580300	-1.42436600
C	0.46842000	-4.45354000	-2.60442900
C	0.69566100	-2.16543200	-3.49167400
C	1.55180900	-1.07889400	-3.04111300
C	2.67029500	-1.65406600	-2.32115000
C	3.17314500	-1.00030600	-1.18139200
C	3.52847700	-1.77249800	0.00000000
C	3.37248600	-3.15877700	0.00000000
C	2.00269400	-4.91621100	0.72903000
C	0.82998100	-5.22580300	1.42436600
C	-0.38514500	-5.54742200	0.70276700
C	-0.38514500	-5.54742200	-0.70276700
C	-1.49899800	-4.96703000	-1.42400900
C	-0.97523600	-4.29288000	-2.60459900
C	-1.54626700	-3.09737800	-3.04148800
C	-0.69122000	-2.01201000	-3.49359500
C	0.97831300	0.12460700	-2.61308300
C	-0.46221000	0.28509300	-2.61595300
C	-1.28711300	-0.76357000	-3.04093000
C	-2.50896000	-1.07934600	-2.32406400
C	-2.66689600	-2.51569300	-2.31887100
C	-3.16938100	-3.16636900	-1.18057100
C	-2.57584000	-4.40670400	-0.72931800
C	-2.57584000	-4.40670400	0.72931800
C	-1.49899800	-4.96703000	1.42400900
C	2.85457300	-3.83545200	1.17939100
C	0.46842000	-4.45354000	2.60442900
C	1.29013700	-3.41337200	-3.04040000
Li	-0.28242600	-0.57660200	0.00000000

BF₄ at B3LYP/6-31G* level

B	-0.00027800	-0.18552200	0.13121600
Br	-0.00117000	-0.04807700	2.07900000
Br	-0.00112700	-1.97631500	-0.64759800
Br	-1.42958700	1.10600800	-0.78206400
Br	1.43216200	1.10390500	-0.78055400

BCl₄ at B3LYP/6-31G* level

B	0.00003200	-0.17608400	0.12449900
Cl	-0.00007800	-1.80922500	-0.59301000
Cl	-1.31638300	1.01400300	-0.71738400
Cl	1.31629100	1.01395600	-0.71753400
Cl	0.00013800	-0.04265000	1.90342800

BBr₄ at B3LYP/6-31G(d) level

B	-0.28782600	0.00000000	0.00002700
Br	-1.27302500	-1.66789500	-0.00000200
Br	-1.27300800	1.66790600	-0.00000400
Br	1.29357200	-0.00000400	1.41745800
Br	1.29357900	-0.00000700	-1.41745600