Electronic Supplementary Material (ESI) for ChemComm.

B_{18}^{2-}: The non-planar member of the Wankel Motor Family

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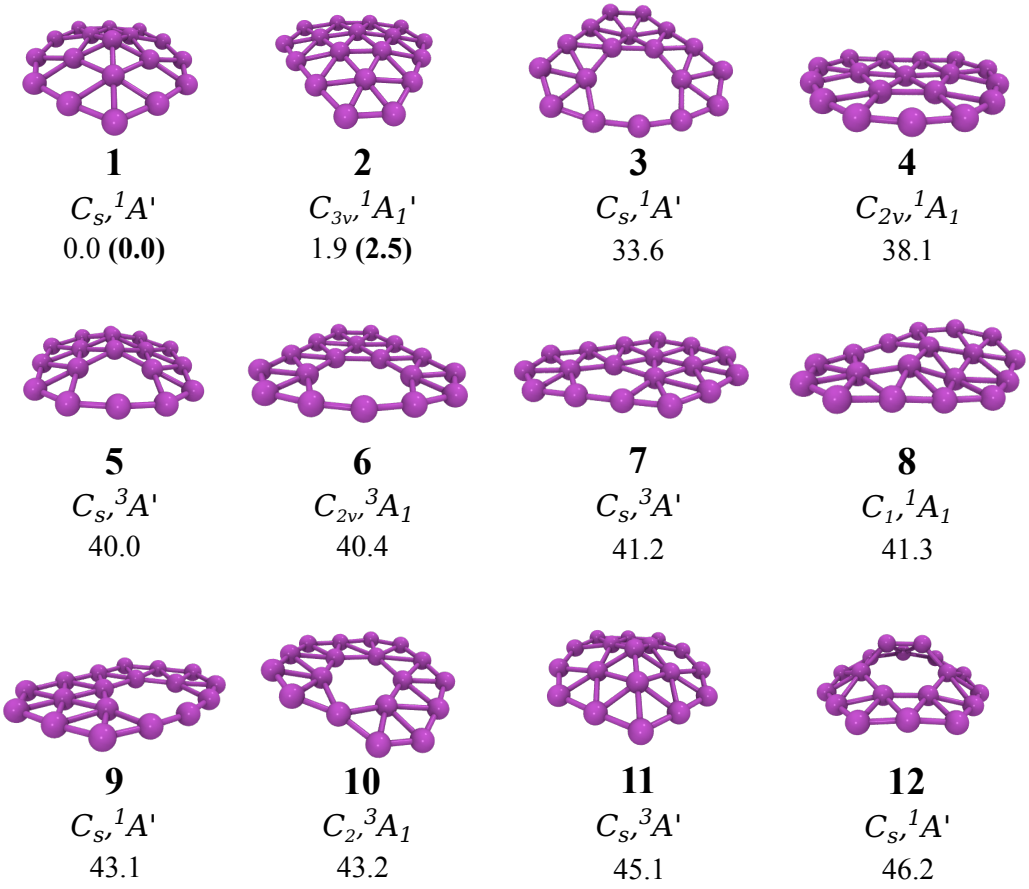

Figure 1-SI. Most stable structures of B_{18}^{2-} and their relative energies (kcal/mol) computed at the TPSS/def2-TZVP level, including ZPE energy. The relative energies computed at the CCSD(T)/def2-TZVP level are given in parentheses.

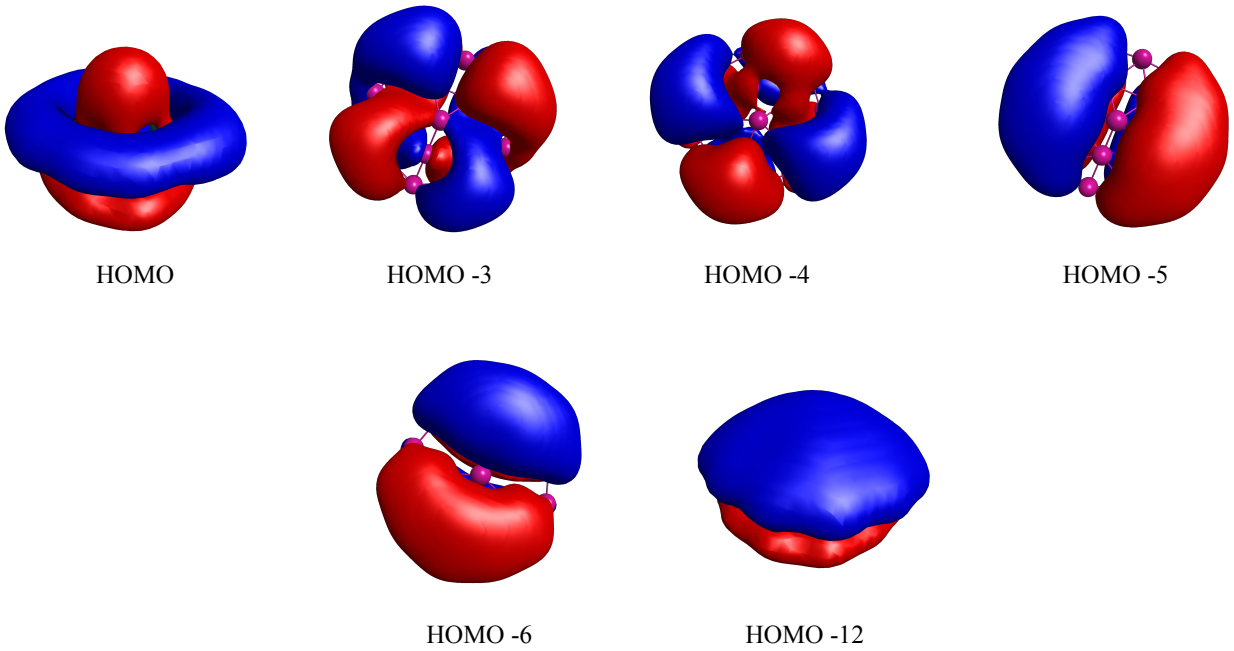

Figure 2-SI. The π-molecular orbitals of the B_{18}^{2-} cluster.

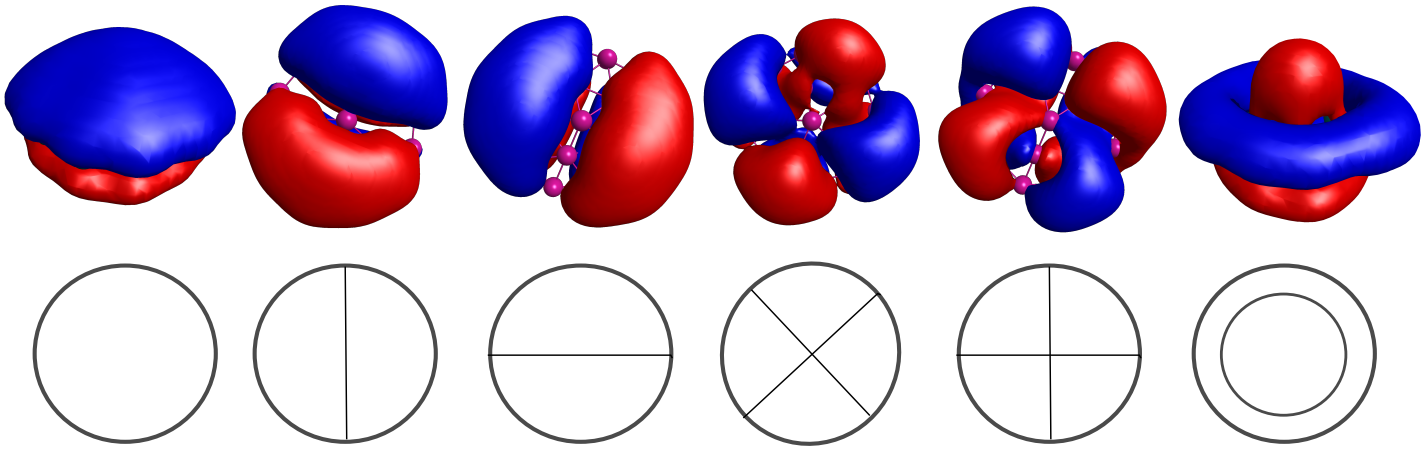

Figure 3-SI. Shapes of the valence π-orbitals of the B_{18}^{2-} cluster and the lowest wave functions for particle in circular box.

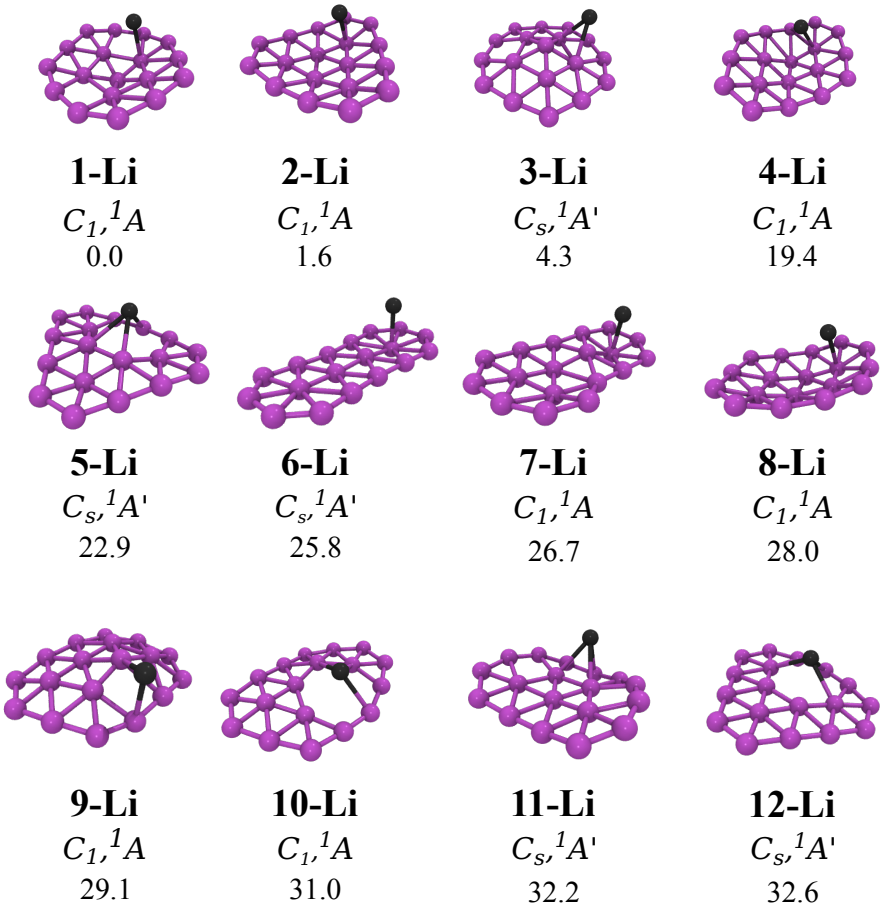

Figure 4-SI. Most stable structures of LiB_{18}^- and their relative energies (kcal/mol) computed at the TPSS/def2-TZVP level, including ZPE energy.

Table 1-SI. The vertical electron detachment energy (VEDE in eV) calculated by Koopmans' theorem (KT), ΔSCF technique and OVGF method, adiabatic electron dissociation energy (AEDE in eV). The basis set in all cases is def2-TZVP.

Levels	VEDE		AEDE	OVGF
	KT	ΔSCF		
TPSS	-1.534	0.284	0.104	0.503
B3LYP	-1.072	0.306	0.135	0.525
PBE0	-0.822	0.401	0.219	0.518
M05-2X	0.075	0.543	0.365	0.542
ωB97X-D	0.683	0.450	0.223	0.570
MP2	0.202	1.044	0.855	0.480

The Cartesian coordinates of the optimized geometries studied at TPSS/def2-TZVP level

B_{18}^{2-} (C_s) (global minimum geometry)

```
-2 1
B     -2.45666000   -0.15854300    1.43832100
B      1.50819400   -0.14536900    2.58025100
B      1.50819400   -0.14536900   -2.58025100
B     -2.45666000   -0.15854300   -1.43832100
B     -0.54111700    0.24653300    1.47080800
B      1.27758600    0.24179300   -0.89004600
B     -1.55514200    0.25878700    0.00000000
B     -0.02906300   -0.13597700    3.07379600
B      1.27758600    0.24179300    0.89004600
B      2.69984200   -0.19826300   -1.59620100
B     -0.00063900    0.75187600    0.00000000
B     -1.52685300   -0.16010400   -2.75590800
B      2.69984200   -0.19826300    1.59620100
B     -3.11651400   -0.23337300    0.00000000
B     -0.54111700    0.24653300   -1.47080800
B     -1.52685300   -0.16010400    2.75590800
B     -0.02906300   -0.13597700   -3.07379600
B      2.80843600   -0.15743200    0.00000000
```

B_{18}^{-2} (C_s) (TS for rotation)

```
-2 1
B       0.24946700    0.46319900    1.48114400
B       0.24531800   -1.23648500   -0.96346900
B       0.24557300    1.56100500    0.00000000
B       0.24531800   -1.23648500    0.96346900
B       0.24946700    0.46319900   -1.48114400
B      -0.14182500    3.02925800    0.76328900
B      -0.15888000   -0.73926300    2.71828500
B      -0.17921600   -2.25935300   -2.19360300
B      -0.15379600    2.06347900   -2.05480000
B      -0.22156800    0.82648200    3.00990100
B      -0.13858200   -2.92568700   -0.80774400
B       0.75259100   -0.00426500    0.00000000
B      -0.22156800    0.82648200   -3.00990100
B      -0.17921600   -2.25935300    2.19360300
B      -0.14182500    3.02925800   -0.76328900
B      -0.15379600    2.06347900    2.05480000
B      -0.15888000   -0.73926300   -2.71828500
B      -0.13858200   -2.92568700    0.80774400
```

B_{18}^{2-} (C_{2v}) (TS for inversion)

```
-2 1
B       0.00000000    1.62336500   -2.75286000
B       0.00000000    3.09879200    0.02929400
B       0.00000000    0.00000000   -0.00146500
B       0.00000000   -1.62336500   -2.75286000
B       0.00000000    0.89263400   -1.30361300
B       0.00000000    0.00000000    1.57187800
B       0.00000000   -0.89263400   -1.30361300
B       0.00000000    2.60930800   -1.53686800
B       0.00000000    1.47761600    0.56608900
B       0.00000000   -1.45949700    2.50712100
B       0.00000000   -2.79375100    1.54858500
B       0.00000000   -1.47761600    0.56608900
B       0.00000000    2.79375100    1.54858500
B       0.00000000    0.00000000   -2.87160500
B       0.00000000   -2.60930800   -1.53686800
B       0.00000000    1.45949700    2.50712100
B       0.00000000   -3.09879200    0.02929400
B       0.00000000    0.00000000    3.18569600
```

LiB_{18}^{-} (C_1) (global minimum geometry)

-1 1

Li	-1.38145900	-0.04544700	-1.58593800
B	-1.67903400	-2.24701100	-0.11864200
B	0.06073100	0.00190700	0.91039900
B	0.38288400	2.74165500	-0.22868500
B	2.60065700	-1.82203100	-0.18483800
B	-2.33977900	1.77702400	-0.09688900
B	1.45740900	-0.72332200	0.35436300
B	1.17376600	-2.54750900	-0.24750400
B	1.08391500	1.18615400	0.36050100
B	-3.01686900	0.33246700	0.08124200
B	-2.87378600	-1.18483100	0.02187600
B	-0.68030800	1.35766700	0.30703800
B	-1.49162600	-0.38903700	0.60147900
B	-0.13635300	-1.51301000	0.28196300
B	-0.33167700	-3.01190200	-0.37580900
B	3.10069000	-0.38553600	-0.07761800
B	2.78362000	1.18659300	-0.08690100
B	1.94688100	2.47197300	-0.22190100
B	-1.21224700	2.79601700	-0.32851200