Electronic Supplementary Information

B_{38}: An All-boron Fullerene Analogue

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Table SI. Optimized atomic coordinates for the B_{38} fullerene analogue.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
B	-0.3723	-2.5176	1.2068	B	3.1618	-0.4495	0.0895
B	-1.1245	2.5210	-0.3462	B	0.2119	1.9134	2.0397
B	1.7538	1.5103	-1.6050	B	-2.1654	1.3800	-1.0710
B	0.0476	-0.3602	-2.7931	B	-2.4214	0.0643	1.3784
B	1.1285	-2.6786	-1.3263	B	0.3723	2.5176	-1.2068
B	1.1245	-2.5210	0.3462	B	-3.1618	0.4495	-0.0895
B	-1.0489	2.2046	-1.9648	B	2.2748	-1.6585	-0.6557
B	0.3706	2.7291	0.5264	B	-1.7539	-1.5104	1.6051
B	-1.3806	1.2053	2.0931	B	-2.5641	-1.1298	0.1058
B	1.4462	0.9743	2.5527	B	1.5397	0.3173	-2.7110
B	2.4214	-0.0643	-1.3684	B	-0.2185	-1.9134	-2.0386
B	-1.4462	-0.9743	-2.5528	B	-1.5397	-0.3173	2.7110
B	-1.1285	2.6786	1.3263	B	-0.3706	-2.7291	-0.5265
B	-1.7487	-2.5282	0.3282	B	-2.2748	1.6585	0.6557
B	2.4053	0.3142	1.4064	B	1.3806	-1.2053	-2.0931
B	2.1654	-1.3800	1.0710	B	-1.3339	0.6471	-2.3949
B	1.7487	2.5282	-0.3282	B	-0.0476	0.3602	2.7931
B	-2.4153	-0.3142	-1.4064	B	2.5641	1.1298	-0.1058
B	1.3339	-0.6471	2.4064	B	1.0489	-2.2046	1.9648

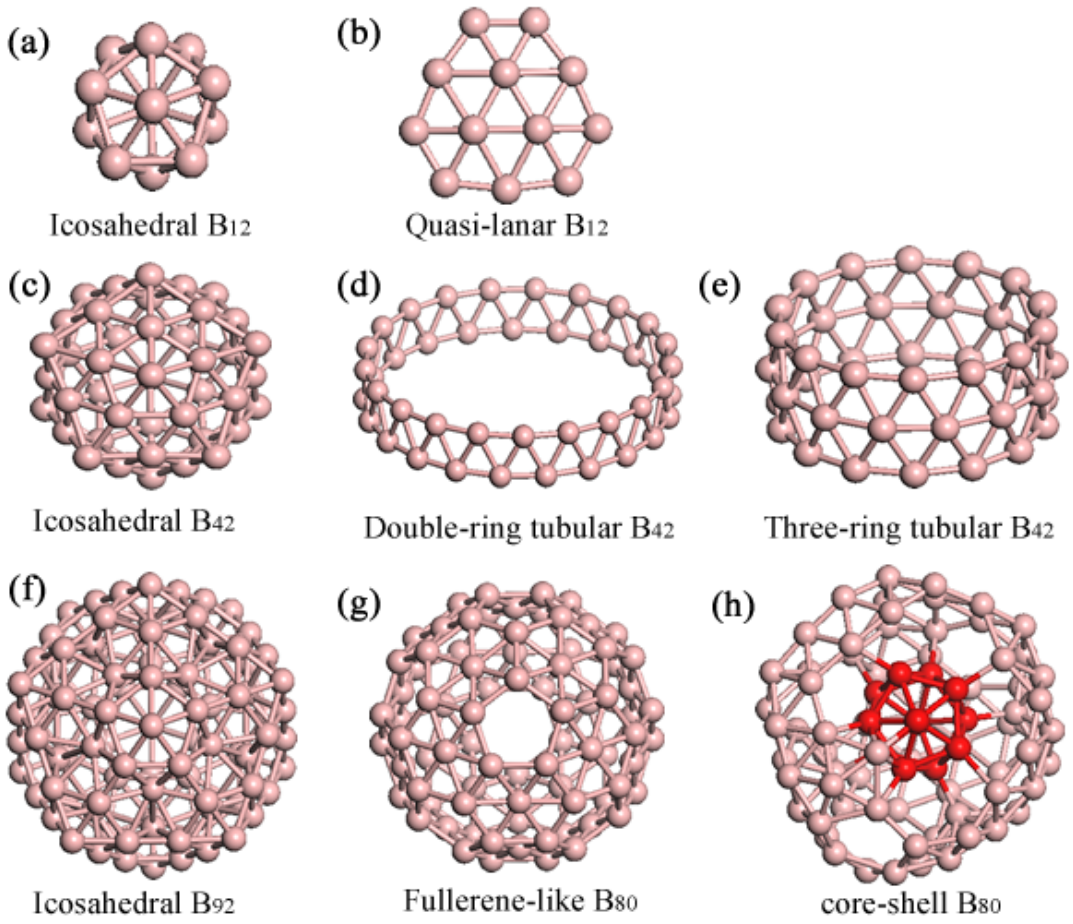

Fig. S1 Stabilities of the icosahedral motifs in B clusters. Mackay icosahedral clusters dependent on the sizes can be represented by 12, 42 and 92 atoms, respectively. The icosahedral B_{12} (a) is already known in bulk materials, but in free-standing clusters it is metastable when compared to the quasi-planar cluster (b)[1]. For B_{42} icosahedral cluster (c), it is energetically less stable than the DRT (d) and TRT structures (e) by about 2.71 and 5.46 eV at PBE0/6-311G* level of theory, respectively. The B_{80} fullerene (g) can be seen as the icosahedral-type structure by removal of 12 vertices atoms of icosahedral B_{92} (f). However, this structure is less stable than the core-shell structure (h)[2]. Therefore, known studies did not establish the phase stabilities of icosahedral structural motifs in free-standing B clusters. They are overwhelmed by the planar, tubular (DRT and TRT) and core-shell structures in different size ranges.

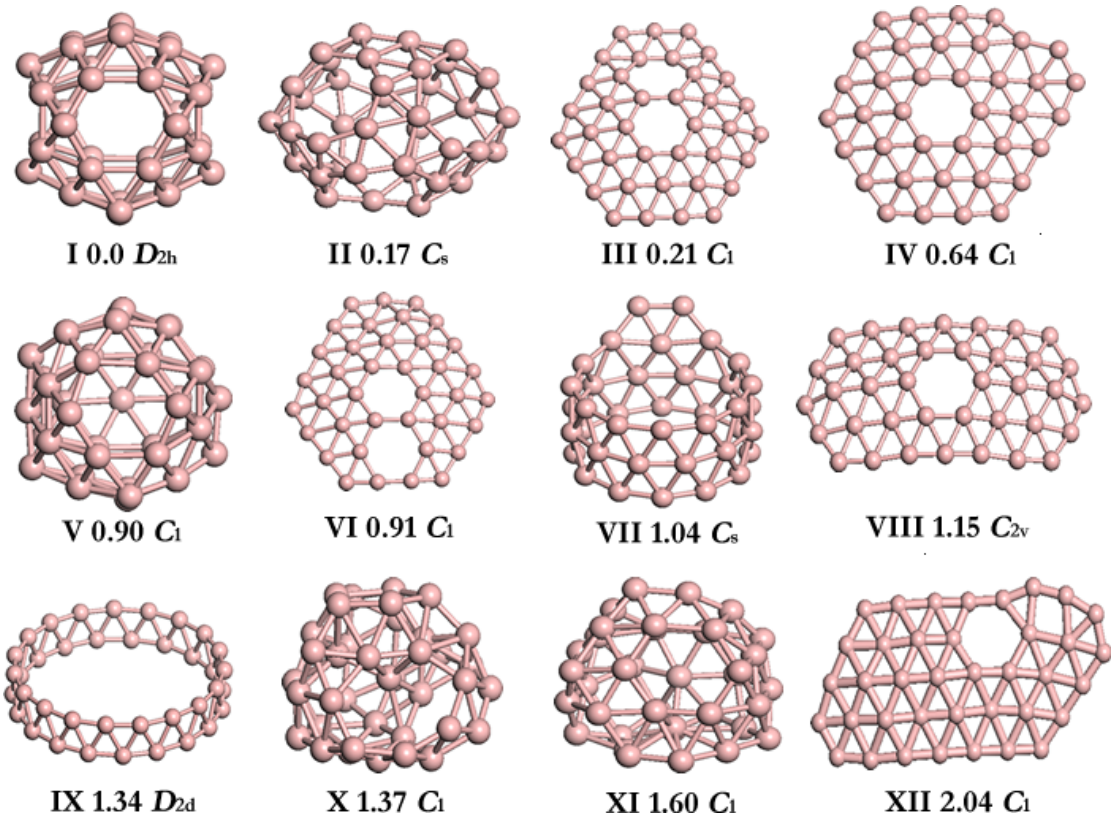

Fig. S2 Structures of low-lying isomers of B_{38}. Bottom labels are point-group symmetries and relative energies to the ground state at PBE0/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

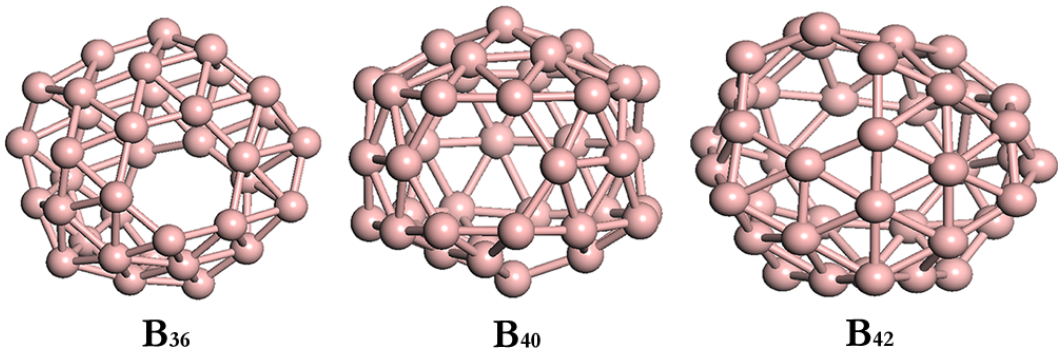

Fig. S3 Lowest-energy cage structures of B_{36}, B_{40} and B_{42} clusters derived from constrained structure searches.

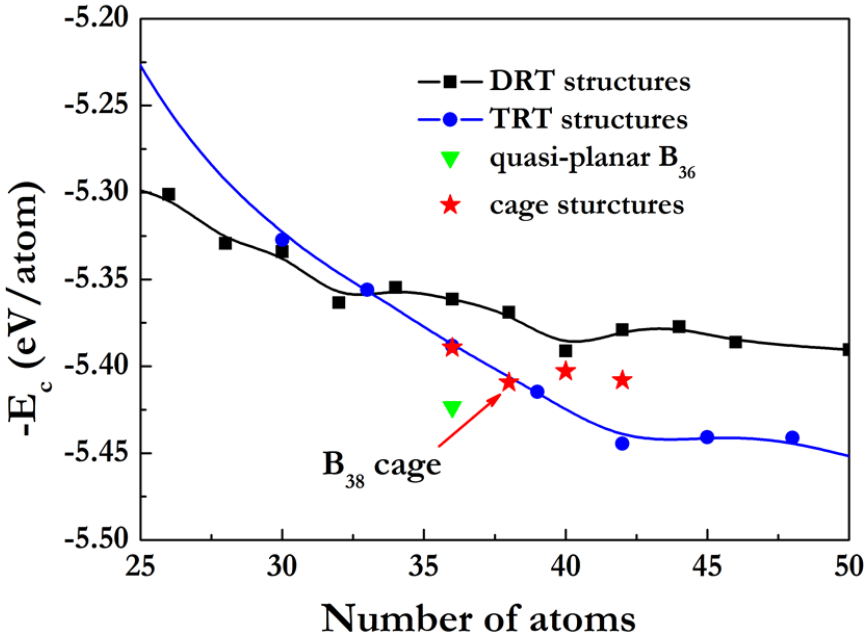

Fig. S4 Cohesive energies (E_c) of representative structures as a function of the number of atoms.

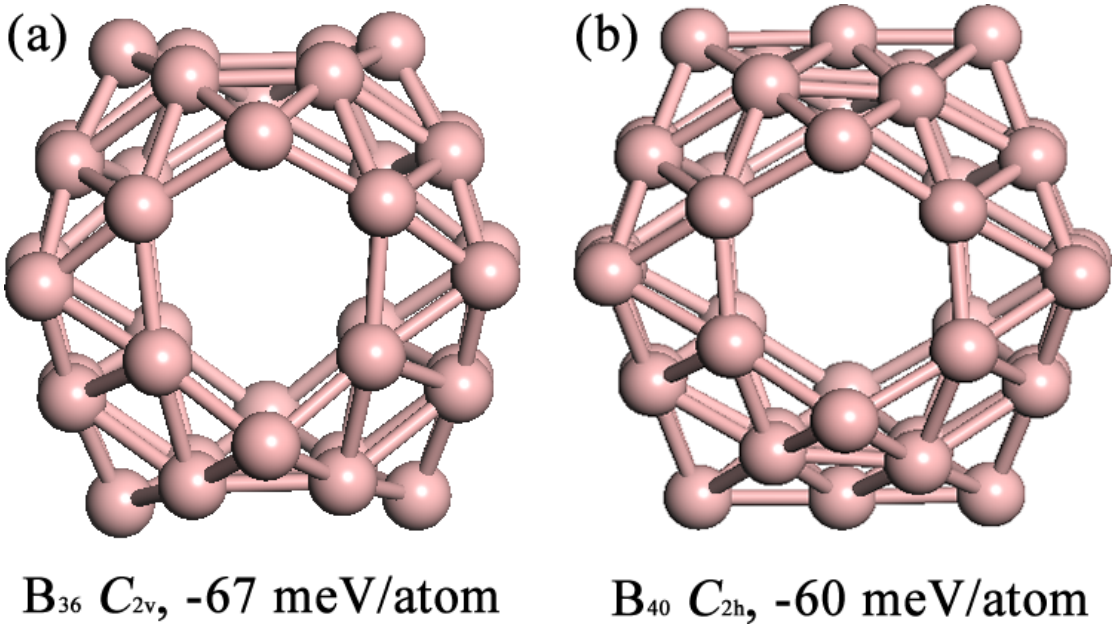

Fig. S5 (a) Model structure of B_{36} cage derived by removing two centered B atoms out of two filled hexagons in B_{38} fullerene analogue, and (b) model structure of B_{40} cage derived by adding two B atoms to each center of the two opposite open hexagons of the B_{38} fullerene analogue. Labels are point-group symmetries and relative cohesive energies to that of the B_{38} fullerene analogue.

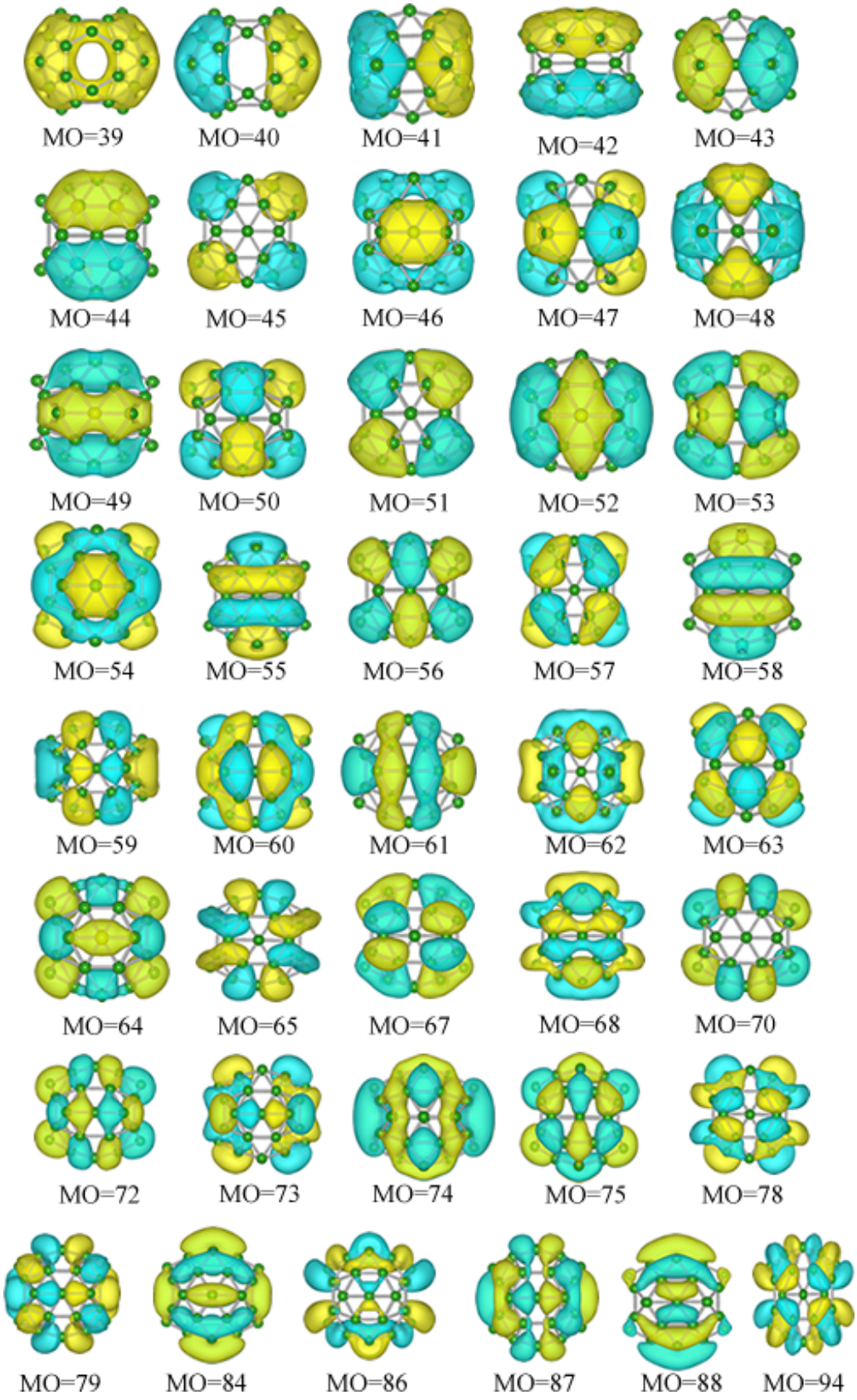

Fig. S6 The 41 σ- canonical molecular orbitals of the B_{38} fullerene analogue.

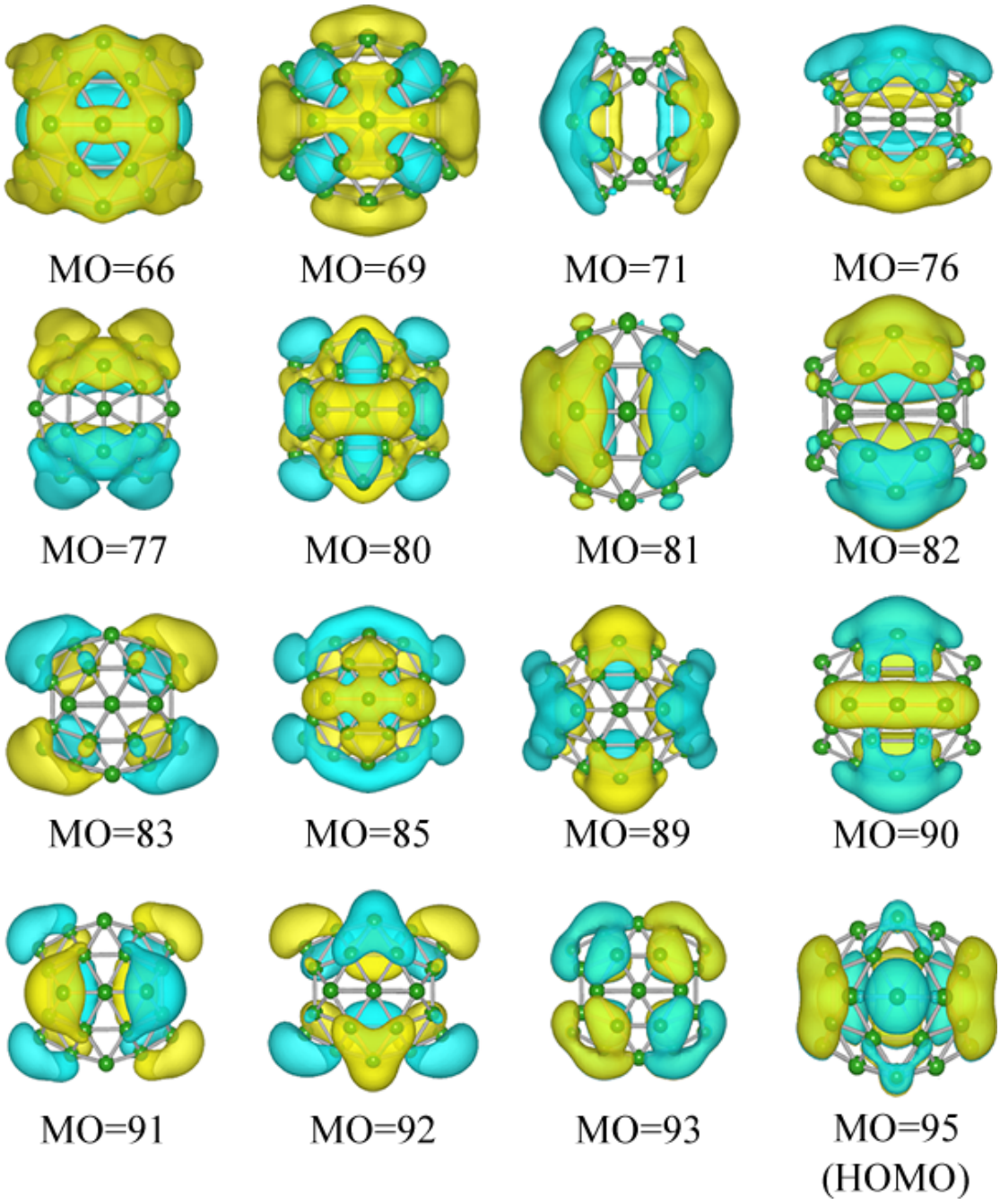

Fig. S7 The 16 π- canonical molecular orbitals of the B_{38} fullerene analogue.

References

1 H.-J. Zhai, B. Kiran, J. Li, and L.-S. Wang, *Nat. Mater.*, 2003, **2**, 827-833.

2 F. Li, P. Jin, D.-e. Jiang, L. Wang, S. B. Zhang, J. Zhao, and Z. Chen, *J. Chem. Phys.*, 2012, **136**, 074302-074309.