Supporting Information

Boron Buckminsterfullerene

Hyun Wook Choi, Yang-Yang Zhang, Deniz Kahraman, Cong-Qiao Xu, Han-Wen Gao, Jun Li, and Lai-Sheng Wang

Corresponding authors: Jun Li, junli@tsinghua.edu.cn; Lai-Sheng Wang, lai-sheng_wang@brown.edu

The PDF file includes:

- Experimental and computational methods
- Figures S1 to S10
- Tables S1 to S12
- References

Experimental and computational methods

***Photoelectron spectroscopy*.** The experiment was conducted on an apparatus, consisting of a laser vaporization supersonic cluster source, a time-of-flight (TOF) mass spectrometer, and a magnetic-bottle type PES apparatus. Details of the apparatus can be found elsewhere.[1] Clusters were produced by directing an intense laser pulse onto a disk target made of ^{11}B-enriched boron powder (97% isotopic purity). The laser-induced plasma was quenched by a high-pressure helium carrier gas seeded with 20% argon, initiating nucleation. Clusters formed inside the nozzle were entrained in the carrier gas and underwent a supersonic expansion to create cold clusters. After passing a skimmer, the collimated cluster beam traveled to the extraction zone of the TOF mass spectrometer. Negatively charged boron clusters (B_n^-) were extracted perpendicularly into the free flight zone of the TOF mass analyzer. The B_{80}^- cluster was mass selected and decelerated before being photodetached by a 193 nm (6.424 eV) laser beam from an ArF excimer laser. More than 90% of the photoelectrons emitted in all 4π solid angles were collimated by a magnetic-bottle and analyzed in a 3.5 m long TOF tube. The electron kinetic energies were calibrated by the known spectrum of the Bi^- atomic anion. The kinetic energy (Ke) resolution ($\Delta Ke/Ke$) of the magnetic-bottle analyzer was 2.5% or ~25 meV for 1 eV electrons.

***Theoretical and computational methods*.** The global-minimum structural searches of the anionic B_{80}^- and neutral B_{80} clusters were performed using the constrained basin-hopping algorithm in the TGMin (v3.0) program,[2-4] interfaced with the Gaussian 16 package.[5] The geometries of the isomers were re-optimized using the generalized gradient approximation (GGA) with the hybrid B3LYP functional[6,7] and split-valence double-zeta plus polarization 6-31G(d) basis sets.[8] In total, 5284 local minima were explored. Vibrational frequency calculations were performed to confirm the true minima on the potential energy surfaces. Then, selected low-lying isomers are re-optimized with a variety of different DFT functionals and the 6-31G(d) basis set.[9] The buckyball isomer was re-optimized at the MP2 level with the resolution-of-the-identity (RI) approximation and the 6-31G(d) basis set[10] by using the ORCA package.[11]

To compare with experimental data, we computed the vertical detachment energies (VDEs) for selected isomers of B_{80}^{-} using the generalized Koopman theory using the Multiwfn package. The computed VDEs were fitted using unit-area Gaussian functions with a width of 0.15 eV (a ratio of 1 to 3 was used for singlet and triplet final states, respectively). The chemical bonding was analyzed using the Adaptive Natural Density Partitioning (AdNDP)[12] within the Gaussian 16 package, using the B3LYP functional and 6-31G(d) basis sets.

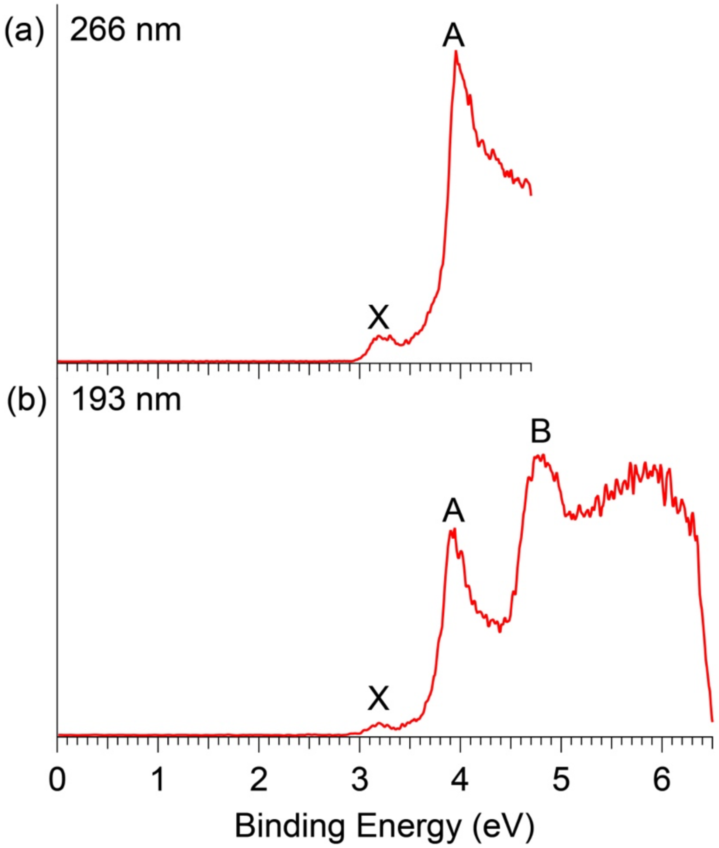
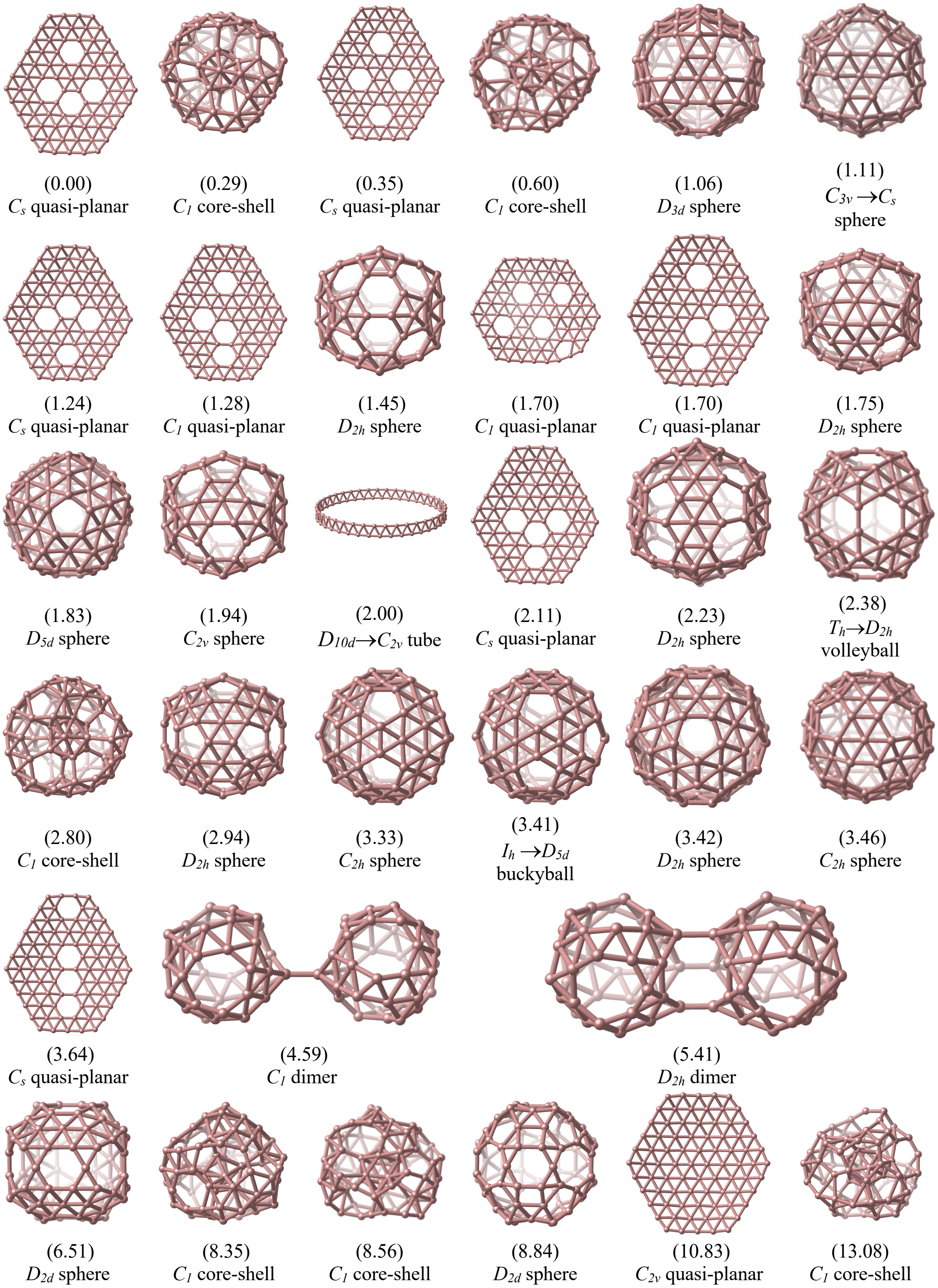


Figure S1. Photoelectron spectroscopy of B_{80}^{-} at (a) 266 nm (4.661 eV) and (b) 193 nm (6.424 eV).



(0.00)
C_s quasi-planar

(0.29)
C_1 core-shell

(0.35)
C_s quasi-planar

(0.60)
C_1 core-shell

(1.06)
D_{3d} sphere

(1.11)
$C_{3v} \rightarrow C_s$
sphere

(1.24)
C_s quasi-planar

(1.28)
C_1 quasi-planar

(1.45)
D_{2h} sphere

(1.70)
C_1 quasi-planar

(1.70)
C_1 quasi-planar

(1.75)
D_{2h} sphere

(1.83)
D_{5d} sphere

(1.94)
C_{2v} sphere

(2.00)
$D_{10d} \rightarrow C_{2v}$ tube

(2.11)
C_s quasi-planar

(2.23)
D_{2h} sphere

(2.38)
$T_h \rightarrow D_{2h}$
volleyball

(2.80)
C_1 core-shell

(2.94)
D_{2h} sphere

(3.33)
C_{2h} sphere

(3.41)
$I_h \rightarrow D_{5d}$
buckyball

(3.42)
D_{2h} sphere

(3.46)
C_{2h} sphere

(3.64)
C_s quasi-planar

(4.59)
C_1 dimer

(5.41)
D_{2h} dimer

(6.51)
D_{2d} sphere

(8.35)
C_1 core-shell

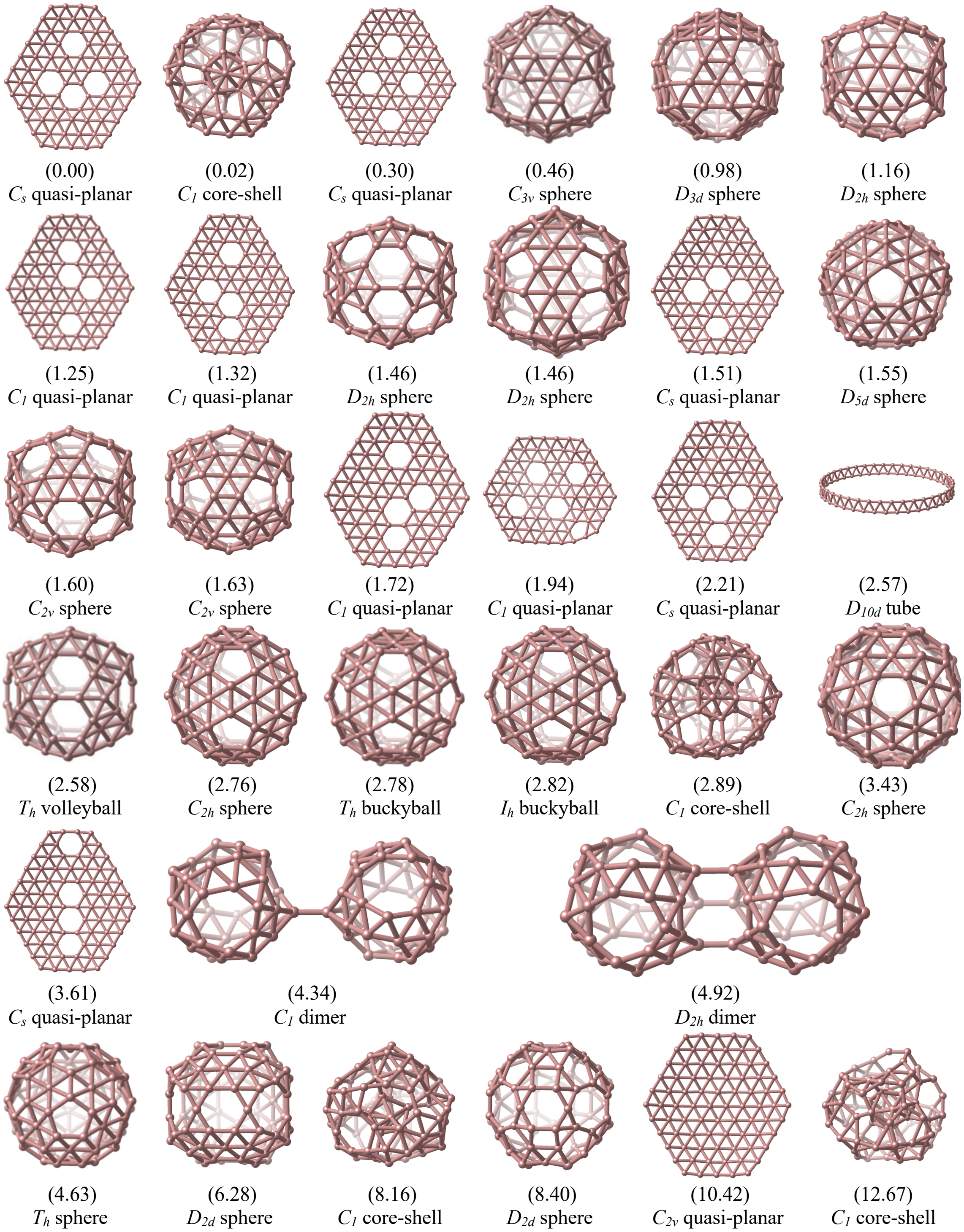
(8.56)
C_1 core-shell

(8.84)
D_{2d} sphere

(10.83)
C_{2v} quasi-planar

(13.08)
C_1 core-shell

Figure S2. Global minimum searches for B_{80}^-. Relative energies (in eV) and symmetries of low-lying isomers of the B_{80}^- anion optimized at the B3LYP/6-31G(d) level. Note that the Jahn-Teller effect reduces the symmetry of the buckyball structure from I_h in the neutral to D_{5d} in the anion.



(0.00)
C_s quasi-planar

(0.02)
C_1 core-shell

(0.30)
C_s quasi-planar

(0.46)
C_{3v} sphere

(0.98)
D_{3d} sphere

(1.16)
D_{2h} sphere

(1.25)
C_1 quasi-planar

(1.32)
C_1 quasi-planar

(1.46)
D_{2h} sphere

(1.46)
D_{2h} sphere

(1.51)
C_s quasi-planar

(1.55)
D_{5d} sphere

(1.60)
C_{2v} sphere

(1.63)
C_{2v} sphere

(1.72)
C_1 quasi-planar

(1.94)
C_1 quasi-planar

(2.21)
C_s quasi-planar

(2.57)
D_{10d} tube

(2.58)
T_h volleyball

(2.76)
C_{2h} sphere

(2.78)
T_h buckyball

(2.82)
I_h buckyball

(2.89)
C_1 core-shell

(3.43)
C_{2h} sphere

(3.61)
C_s quasi-planar

(4.34)
C_1 dimer

(4.92)
D_{2h} dimer

(4.63)
T_h sphere

(6.28)
D_{2d} sphere

(8.16)
C_1 core-shell

(8.40)
D_{2d} sphere

(10.42)
C_{2v} quasi-planar

(12.67)
C_1 core-shell

Fiugre S3. Global minimum searches for B_{80}. Relative energies (in eV) and symmetries of low-lying isomers of neutral B_{80} optimized at the B3LYP/6-31G(d) level.

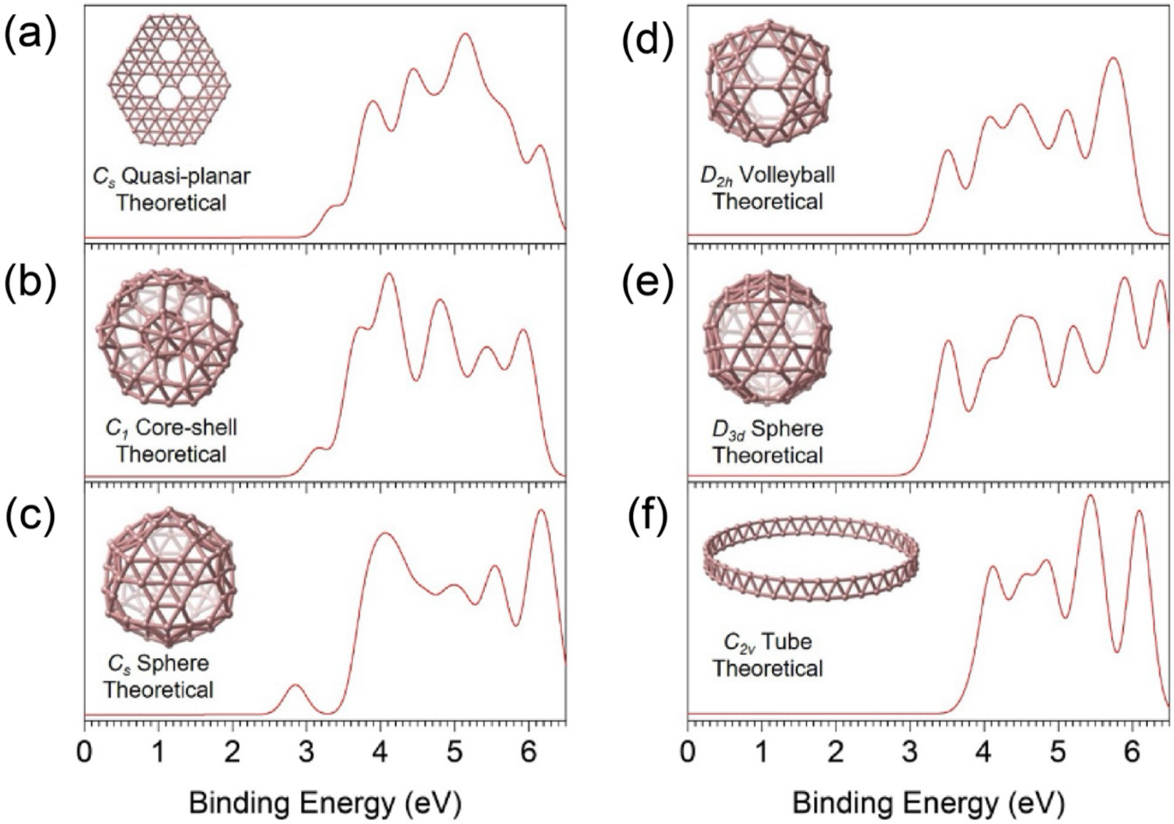


Figure S4. Simulated photoelectron spectra for different structures of B_{80}^{-}. (a) The planar structure. (b) The core-shell structure. (c) The C_s cage structure (corresponding to the neutral C_{3v} cage). (d) The D_{2h} volleyball structure (corresponding to the neutral T_h volleyball structure). (e) The D_{3d} cage structure. (f) The double ring structure.

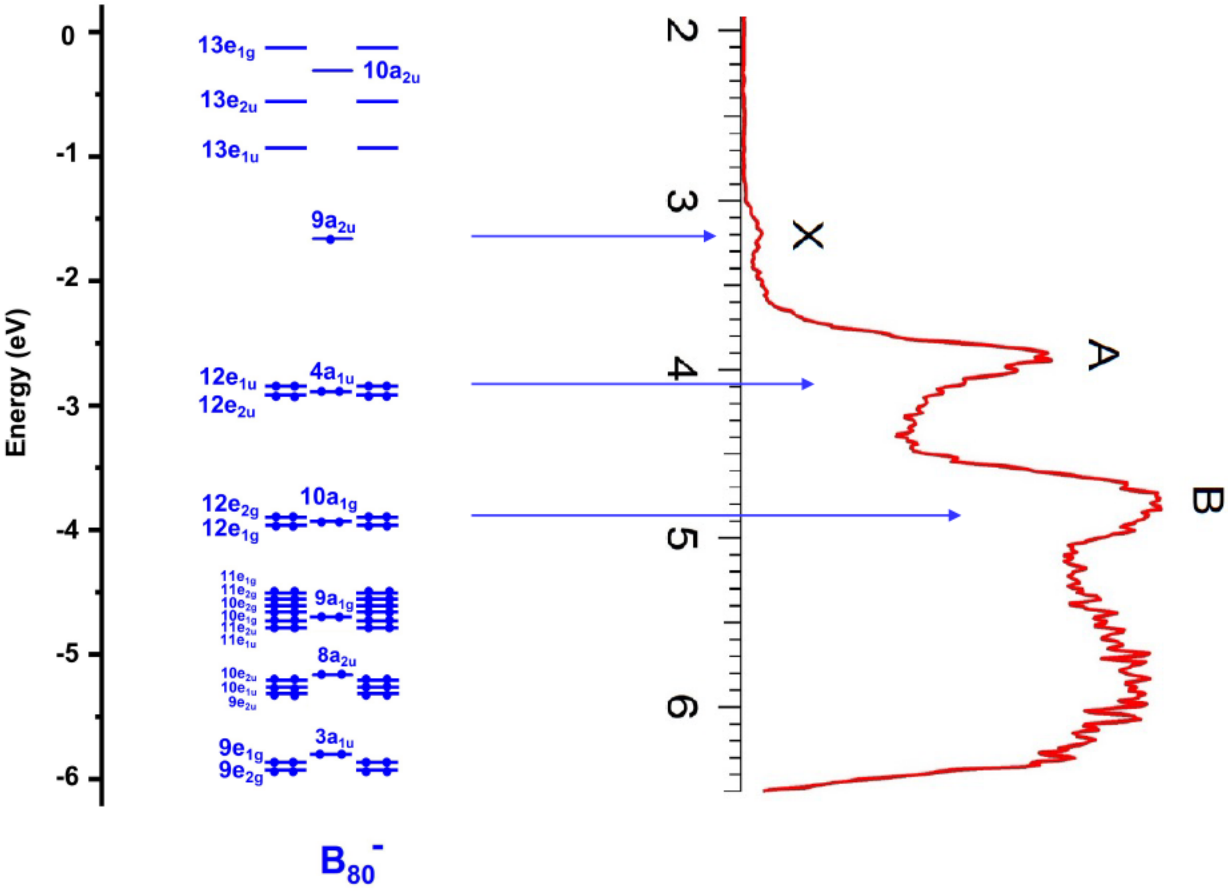
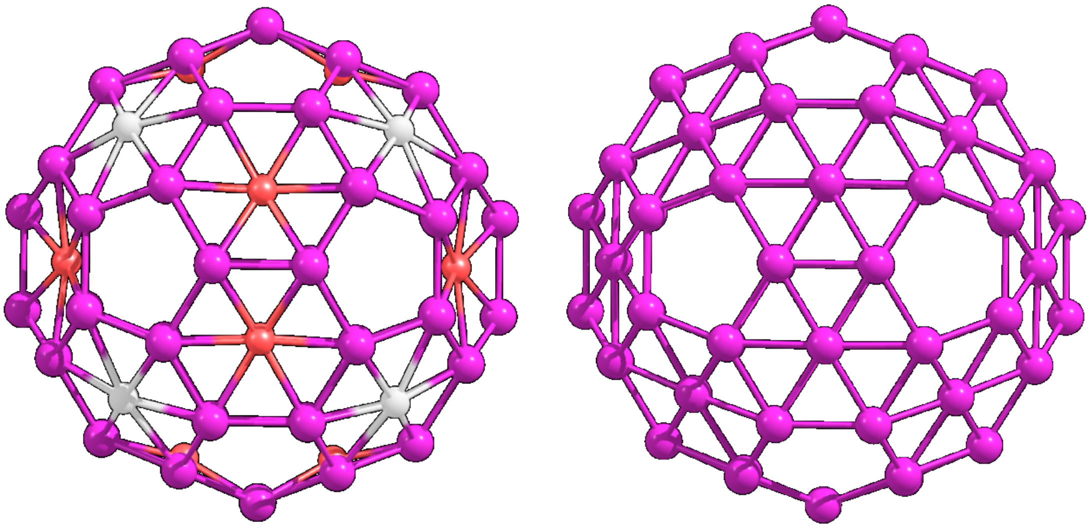
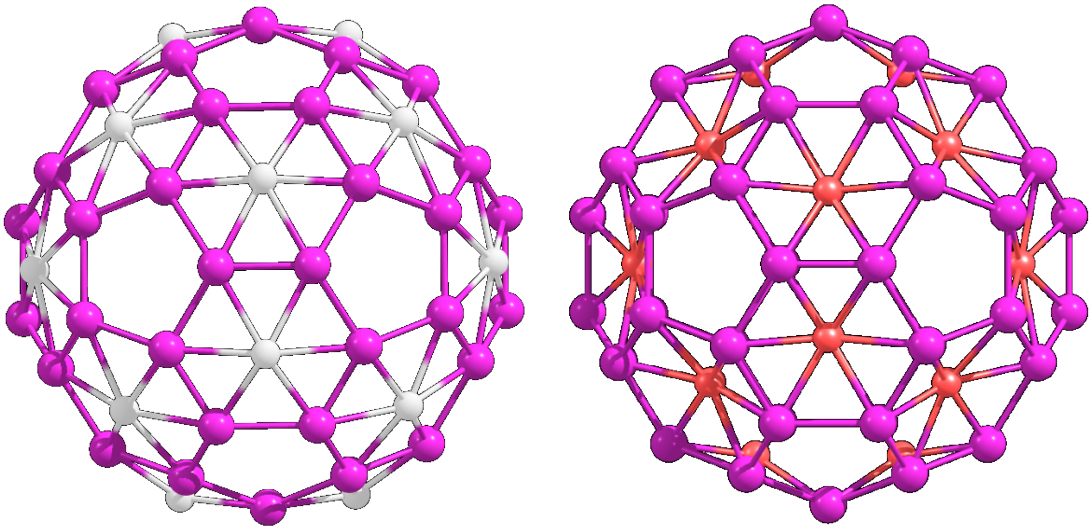


Figure S5. Comparison of the molecular orbital energy levels of B_{80}^- with the 193 nm photoelectron spectrum.



T_h structure

I_h structure



outer-I_h structure

inner-I_h structure

Figure S6. The different symmetries of the B_{80} buckyball. The geometrical structure of T_h and different I_h structures of the B_{80} buckyball. Color codes: white for the protruding B atoms and red for the recessed B atoms.

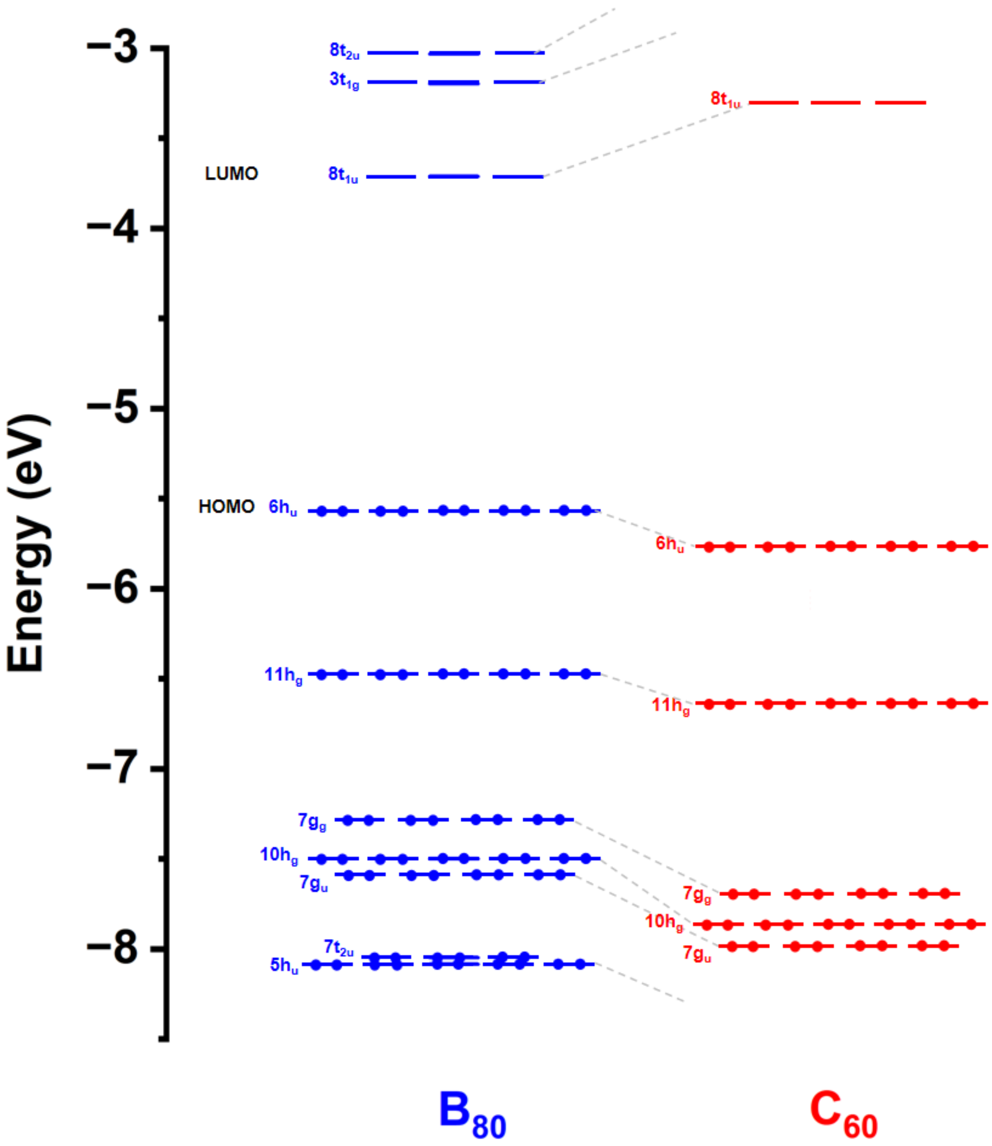


Figure S7. Comparison of the molecular orbital energy levels between the B_{80} and C_{60} buckyballs. The orbital energies (in eV) are computed at the B3LYP/6-31G(d) level with small frozen cores.

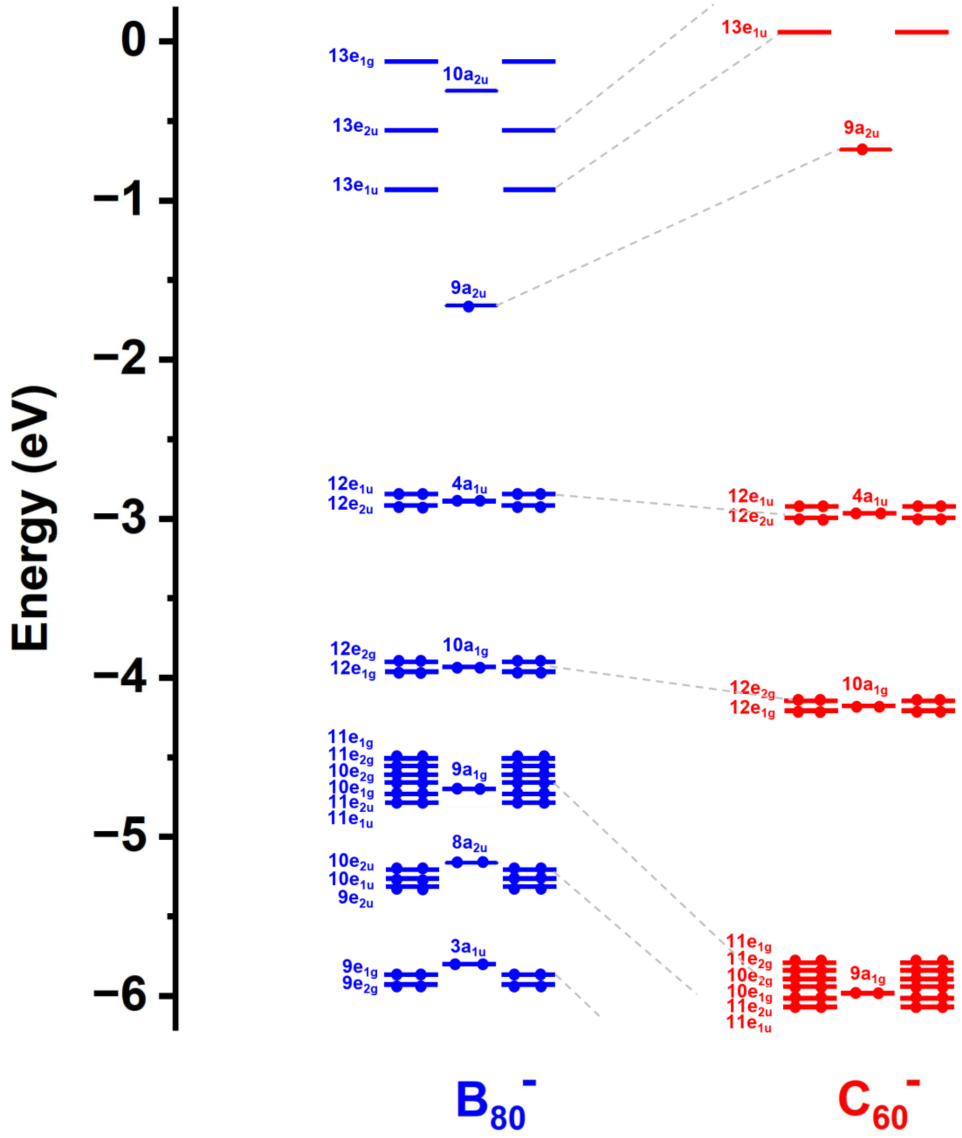


Figure S8. Comparison of the molecular orbital energy levels between B_{80}^{-} and C_{60}^{-}. The orbital energies (in eV) are computed at the at the B3LYP/6-31G(d) level with small frozen cores.

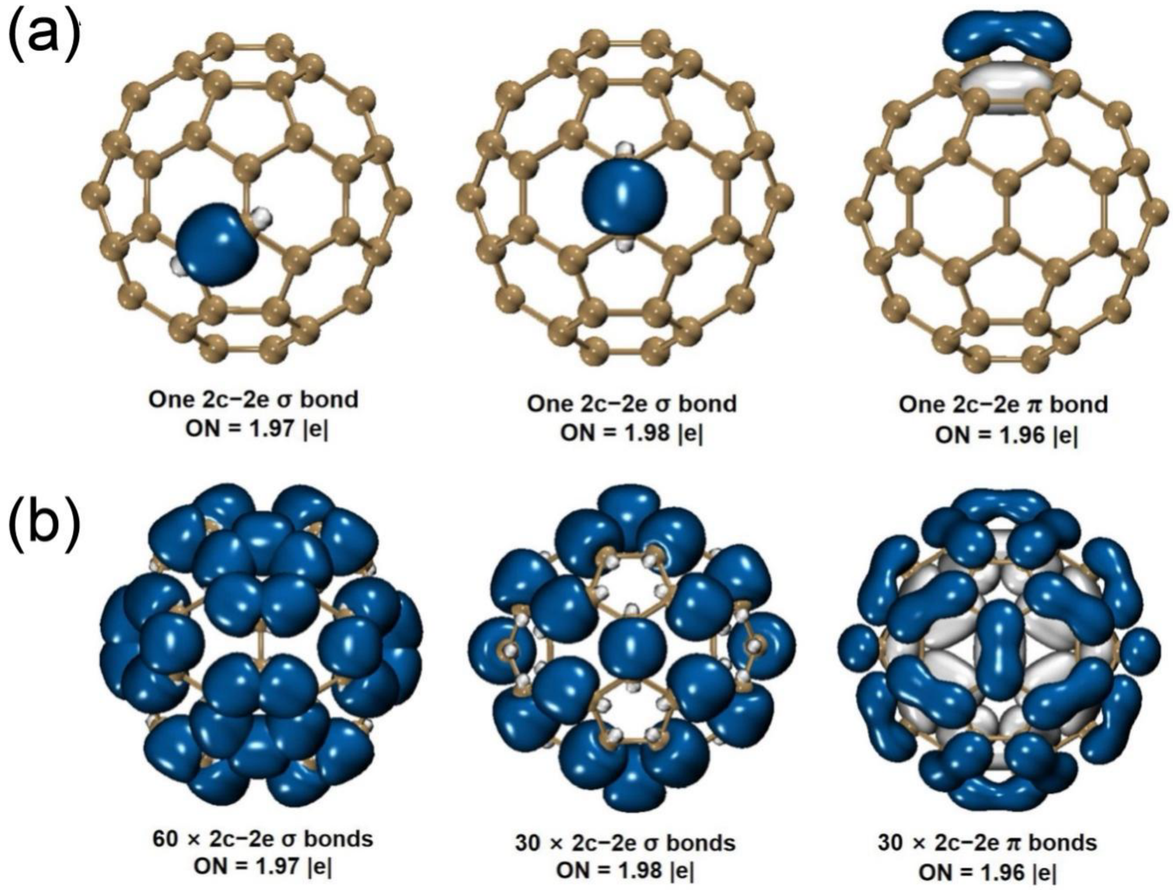


Figure S9. Chemical bonding analyses for the C_{60} buckyball using the AdNDP method at the B3LYP/6-31G(d) level. (a) The three types of two-center-two electron (2c-2e) bonds. (b) Full sets of bonds for the C_{60} buckyball. Isovalue is 0.1 a.u. Note that the 60 2c-2e σ bonds on the left of (b) correspond to the C–C single bonds around the 12 pentagons. The 30 2c-2e σ and π bonds together correspond to the 30 C=C double bonds between the hexagons.

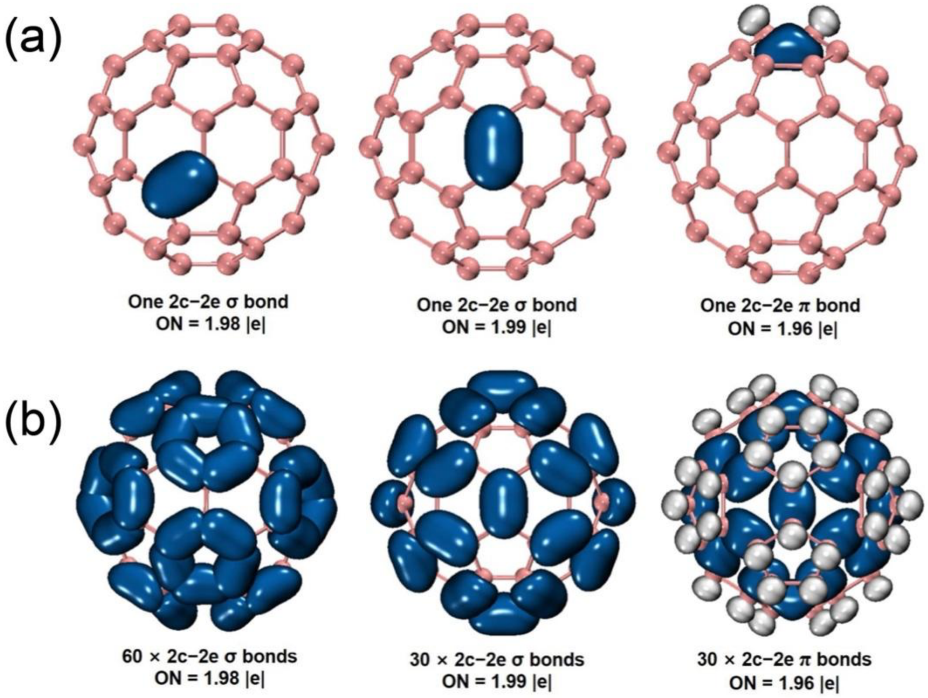


Figure S10. Chemical bonding analyses for the $[B_{60}]^{60-}[X]_{20}^{60+}$ (X is a dummy atom) hypothetical buckyball from AdNDP bonding analyses at the B3LYP/6-31G(d) level. (a) The three types of two-center-two electron (2c-2e) bonds. (b) Full sets of bonds for the $[B_{60}]^{60-}[X]_{20}^{60+}$ buckyball. Isovalue is 0.1 a.u. Note the similarity with that for C_{60} in Fig. S9.

Table S1. The relative energies (in eV) of selected neutral B_{80} optimized at different DFT levels with the 6−31G(d) basis set. The Grimme dispersion correction was abbreviated as D4 by using ORCA package.

Method	Buckyball (I_h)	Core-shell (C_1)	Sphere (D_{3d})	Sphere (C_{3v})	Volleyball (T_h)	Quasi-planar (C_s)	Tube (D_{10d})
LDA	0.000	−3.278	0.317	1.910	2.172	3.946	20.084
M06-2X	0.000	−4.198	0.051	0.109	2.147	1.864	-
wB97X-D4	0.000	−8.489	0.578	0.224	2.846	3.408	14.952
OLYP-D4	0.000	−8.742	0.350	2.094	2.832	3.962	18.701
HF-D4	0.000	−10.444	−0.626	−3.601	−0.256	−1.050	1.675
BLYP-D4	0.000	−5.753	−1.595	−1.563	−0.827	−0.438	6.123
BP86-D4	0.000	−5.682	−0.669	0.183	0.797	1.965	12.787
GLYP-D4	0.000	−8.731	−1.158	−0.686	0.135	1.553	11.092
mPWLYP-D4	0.000	−5.012	−1.689	−1.738	−1.030	−0.861	5.344
PBE-D4	0.000	−4.768	−0.361	0.764	1.298	2.124	14.220
PBE0-D4	0.000	−5.759	−0.094	0.746	2.354	2.494	14.535
PW91-D4	0.000	−4.455	−0.604	0.309	0.856	1.555	12.535
PWP-D4	0.000	−3.532	−0.908	−0.262	0.270	0.768	10.180
REVPBE-D4	0.000	−6.877	−0.230	1.032	1.702	2.659	15.336
RPBE-D4	0.000	−7.020	−0.205	1.090	1.780	2.646	15.448
TPSS-D4	0.000	−6.817	−0.698	0.128	0.906	1.238	11.627
TPSSh-D4	0.000	−6.979	−0.551	0.192	1.373	1.457	11.905
XLYP-D4	0.000	−6.718	−1.516	−1.392	−0.603	0.000	7.606

Table S2. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^{-} (D_{5d}, $^{2}A_{2u}$) buckyball, in comparison with the experimental results. The bold-face indicates the orbitals from which an electron is detached.

Feature	State	Configuration	Theo. VDE [a]	Expt. VDE
X	$^{1}A_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}\mathbf{9a_{2u}^{0}}\}$	3.22	3.2
A	$^{3}E_{1g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}\mathbf{12e_{1u}^{3}}9a_{2u}^{1}\}$	4.15	4.0
	$^{1}E_{1g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}\mathbf{12e_{1u}^{3}}9a_{2u}^{1}\}$	4.18	
	$^{3}A_{2g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}\mathbf{4a_{1u}^{1}}12e_{1u}^{4}9a_{2u}^{1}\}$	4.17	
	$^{1}A_{2g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}\mathbf{4a_{1u}^{1}}12e_{1u}^{4}9a_{2u}^{1}\}$	4.19	
	$^{3}E_{2g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}\mathbf{12e_{2u}^{3}}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	4.22	
	$^{1}E_{2g}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}\mathbf{12e_{2u}^{3}}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	4.24	
B	$^{3}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}\mathbf{12e_{2g}^{3}}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.17	4.8
	$^{1}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}\mathbf{12e_{2g}^{3}}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.19	
	$^{3}A_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}\mathbf{10a_{1g}^{1}}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.20	
	$^{1}A_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}\mathbf{10a_{1g}^{1}}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.22	
	$^{3}E_{1u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}\mathbf{12e_{1g}^{3}}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.24	
	$^{1}E_{1u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}\mathbf{12e_{1g}^{3}}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	5.26	
	$^{3}E_{1u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}\mathbf{11e_{1g}^{3}}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.07	~6.0
	$^{1}E_{1u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}\mathbf{11e_{1g}^{3}}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.09	
	$^{3}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}\mathbf{11e_{2g}^{3}}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.15	
	$^{1}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}10e_{2g}^{4}\mathbf{11e_{2g}^{3}}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.18	
	$^{3}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}\mathbf{10e_{2g}^{3}}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.20	
	$^{1}E_{2u}$	$\{...9a_{1g}^{2}10e_{1g}^{4}\mathbf{10e_{2g}^{3}}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.23	
	$^{3}E_{1u}$	$\{...9a_{1g}^{2}\mathbf{10e_{1g}^{3}}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.27	
	$^{1}E_{1u}$	$\{...9a_{1g}^{2}\mathbf{10e_{1g}^{3}}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.29	
	$^{3}A_{2u}$	$\{\mathbf{...9a_{1g}^{1}}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.32	
	$^{1}A_{2u}$	$\{\mathbf{...9a_{1g}^{1}}10e_{1g}^{4}10e_{2g}^{4}11e_{2g}^{4}11e_{1g}^{4}12e_{1g}^{4}10a_{1g}^{2}12e_{2g}^{4}12e_{2u}^{4}4a_{1u}^{2}12e_{1u}^{4}9a_{2u}^{1}\}$	6.34	

Table S3. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^{-} (C_s, $^{2}A'$) quasi-planar. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE [a]
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}\mathbf{108a'^{0}}\}$	3.35
$^{3}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}\mathbf{107a'^{1}}108a'^{1}\}$	3.77
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}\mathbf{107a'^{1}}108a'^{1}\}$	3.79
$^{3}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}\mathbf{93a''^{1}}107a'^{2}108a'^{1}\}$	3.99
$^{1}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}\mathbf{93a''^{1}}107a'^{2}108a'^{1}\}$	4.02
$^{3}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}\mathbf{106a'^{1}}93a''^{2}107a'^{2}108a'^{1}\}$	4.33
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}\mathbf{106a'^{1}}93a''^{2}107a'^{2}108a'^{1}\}$	4.35
$^{3}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}\mathbf{92a''^{1}}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.48
$^{1}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}\mathbf{92a''^{1}}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.51
$^{3}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}\mathbf{91a''^{1}}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.73
$^{1}A''$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}\mathbf{91a''^{1}}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.75
$^{3}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}\mathbf{105a'^{1}}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.97
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}104a'^{2}\mathbf{105a'^{1}}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	4.99
$^{3}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}\mathbf{104a'^{1}}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.13
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}103a'^{2}\mathbf{104a'^{1}}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.15
$^{3}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}\mathbf{103a'^{1}}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.27
$^{1}A'$	$\{\ldots 89a''^{2}102a'^{2}90a''^{2}\mathbf{103a'^{1}}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.29
$^{3}A''$	$\{\ldots 89a''^{2}102a'^{2}\mathbf{90a''^{1}}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.51
$^{1}A''$	$\{\ldots 89a''^{2}102a'^{2}\mathbf{90a''^{1}}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.53
$^{3}A'$	$\{\ldots 89a''^{2}\mathbf{102a'^{1}}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.76
$^{1}A'$	$\{\ldots 89a''^{2}\mathbf{102a'^{1}}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	5.78
$^{3}A''$	$\{\mathbf{\ldots 89a''^{1}}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	6.16
$^{1}A''$	$\{\mathbf{\ldots 89a''^{1}}102a'^{2}90a''^{2}103a'^{2}104a'^{2}105a'^{2}91a''^{2}92a''^{2}106a'^{2}93a''^{2}107a'^{2}108a'^{1}\}$	6.18

Table S4. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B$_{80}^{-}$ (C_1, ^{2}A) core-shell. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE ^{a}
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2\mathbf{201a^0}\}$	3.15
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2\mathbf{200a^1}201a^1\}$	3.60
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2\mathbf{200a^1}201a^1\}$	3.62
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2\mathbf{199a^1}200a^2201a^1\}$	3.77
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2\mathbf{199a^1}200a^2201a^1\}$	3.79
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2\mathbf{198a^1}199a^2200a^2201a^1\}$	4.05
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2\mathbf{198a^1}199a^2200a^2201a^1\}$	4.08
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2\mathbf{197a^1}198a^2199a^2200a^2201a^1\}$	4.10
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2196a^2\mathbf{197a^1}198a^2199a^2200a^2201a^1\}$	4.12
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2\mathbf{196a^1}197a^2198a^2199a^2200a^2201a^1\}$	4.30
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2195a^2\mathbf{196a^1}197a^2198a^2199a^2200a^2201a^1\}$	4.33
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2\mathbf{195a^1}196a^2197a^2198a^2199a^2200a^2201a^1\}$	4.66
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2194a^2\mathbf{195a^1}196a^2197a^2198a^2199a^2200a^2201a^1\}$	4.68
^{3}A	$\{...189a^2190a^2191a^2192a^2193a^2\mathbf{194a^1}195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	4.80
^{1}A	$\{...189a^2190a^2191a^2192a^2193a^2\mathbf{194a^1}195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	4.82
^{3}A	$\{...189a^2190a^2191a^2192a^2\mathbf{193a^1}194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	4.98
^{1}A	$\{...189a^2190a^2191a^2192a^2\mathbf{193a^1}194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.01
^{3}A	$\{...189a^2190a^2191a^2\mathbf{192a^1}193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.31
^{1}A	$\{...189a^2190a^2191a^2\mathbf{192a^1}193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.34
^{3}A	$\{...189a^2190a^2\mathbf{191a^1}192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.53
^{1}A	$\{...189a^2190a^2\mathbf{191a^1}192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.56
^{3}A	$\{...189a^2\mathbf{190a^1}191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.85
^{1}A	$\{...189a^2\mathbf{190a^1}191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	5.87
^{3}A	$\{...\mathbf{189a^1}190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	6.01
^{1}A	$\{...\mathbf{189a^1}190a^2191a^2192a^2193a^2194a^2195a^2196a^2197a^2198a^2199a^2200a^2201a^1\}$	6.03

Table S5. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^{-} (C_s, $^2A''$) sphere. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE ^{a}
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}\mathbf{89a''^{0}}\}$	2.85
$^3A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}\mathbf{112a'^{1}}89a''^{1}\}$	3.77
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}\mathbf{112a'^{1}}89a''^{1}\}$	3.79
$^3A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}\mathbf{88a''^{1}}112a'^{2}89a''^{1}\}$	3.97
$^1A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}\mathbf{88a''^{1}}112a'^{2}89a''^{1}\}$	3.99
$^3A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}\mathbf{111a'^{1}}88a''^{2}112a'^{2}89a''^{1}\}$	4.14
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}\mathbf{111a'^{1}}88a''^{2}112a'^{2}89a''^{1}\}$	4.16
$^3A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}\mathbf{87a''^{1}}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.34
$^1A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}\mathbf{87a''^{1}}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.36
$^3A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}\mathbf{110a'^{1}}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.60
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}\mathbf{110a'^{1}}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.62
$^3A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}\mathbf{86a''^{1}}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.88
$^1A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}\mathbf{86a''^{1}}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	4.91
$^3A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}\mathbf{85a''^{1}}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.13
$^1A'$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}109a'^{2}\mathbf{85a''^{1}}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.16
$^3A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}\mathbf{109a'^{1}}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.45
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}108a'^{2}\mathbf{109a'^{1}}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.47
$^3A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}\mathbf{108a'^{1}}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.64
$^1A''$	$\{\ldots 106a'^{2}107a'^{2}84a''^{2}\mathbf{108a'^{1}}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	5.66
$^3A'$	$\{\ldots 106a'^{2}107a'^{2}\mathbf{84a''^{1}}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.03
$^1A'$	$\{\ldots 106a'^{2}107a'^{2}\mathbf{84a''^{1}}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.05
$^3A''$	$\{\ldots 106a'^{2}\mathbf{107a'^{1}}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.16
$^1A''$	$\{\ldots 106a'^{2}\mathbf{107a'^{1}}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.18
$^3A''$	$\{\ldots \mathbf{106a'^{1}}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.31
$^1A''$	$\{\ldots \mathbf{106a'^{1}}107a'^{2}84a''^{2}108a'^{2}109a'^{2}85a''^{2}86a''^{2}110a'^{2}87a''^{2}111a'^{2}88a''^{2}112a'^{2}89a''^{1}\}$	6.33

Table S6. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^{-} (D_{2h}, $^{2}B_{2u}$) volleyball. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE [a]
$^{1}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}\mathbf{28b_{2u}^{0}}\}$	3.48
$^{3}B_{2g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}\mathbf{19a_{u}^{1}}28b_{2u}^{1}\}$	3.51
$^{1}B_{2g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}\mathbf{19a_{u}^{1}}28b_{2u}^{1}\}$	3.53
$^{3}B_{2g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}\mathbf{18a_{u}^{1}}19a_{u}^{2}28b_{2u}^{1}\}$	3.97
$^{1}B_{2g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}\mathbf{18a_{u}^{1}}19a_{u}^{2}28b_{2u}^{1}\}$	3.99
$^{3}A_{g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}\mathbf{27b_{2u}^{1}}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.12
$^{1}A_{g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}\mathbf{27b_{2u}^{1}}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.14
$^{3}B_{1g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}\mathbf{27b_{3u}^{1}}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.39
$^{1}B_{1g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}\mathbf{27b_{3u}^{1}}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.42
$^{3}B_{3g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}\mathbf{27b_{1u}^{1}}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.53
$^{1}B_{3g}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}\mathbf{27b_{1u}^{1}}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.55
$^{3}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}\mathbf{34a_{g}^{1}}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.75
$^{1}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}\mathbf{34a_{g}^{1}}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	4.77
$^{3}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}\mathbf{33a_{g}^{1}}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.07
$^{1}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}\mathbf{33a_{g}^{1}}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.09
$^{3}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}\mathbf{32a_{g}^{1}}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.17
$^{1}B_{2u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}\mathbf{32a_{g}^{1}}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.19
$^{3}A_{u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}\mathbf{22b_{2g}^{1}}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.55
$^{1}A_{u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}22b_{1g}^{2}\mathbf{22b_{2g}^{1}}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.57
$^{3}B_{3u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}\mathbf{22b_{1g}^{1}}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.66
$^{1}B_{3u}$	$\{...26b_{1u}^{2}22b_{3g}^{2}\mathbf{22b_{1g}^{1}}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.68
$^{3}B_{1u}$	$\{...26b_{1u}^{2}\mathbf{22b_{3g}^{1}}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.81
$^{1}B_{1u}$	$\{...26b_{1u}^{2}\mathbf{22b_{3g}^{1}}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.83
$^{3}B_{3g}$	$\{...\mathbf{26b_{1u}^{1}}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.90
$^{1}B_{3g}$	$\{...\mathbf{26b_{1u}^{1}}22b_{3g}^{2}22b_{1g}^{2}22b_{2g}^{2}32a_{g}^{2}33a_{g}^{2}34a_{g}^{2}27b_{1u}^{2}27b_{3u}^{2}27b_{2u}^{2}18a_{u}^{2}19a_{u}^{2}28b_{2u}^{1}\}$	5.92

Table S7. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^{-} (D_{3d}, $^{2}A_{1u}$) sphere, in comparison with the experimental results. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE [a]
$^{1}A_{1u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}\mathbf{3a_{1u}^{0}}\}$	3.28
$^{3}E_{g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}\mathbf{33e_{u}^{3}}3a_{1u}^{1}\}$	3.52
$^{1}E_{g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}\mathbf{33e_{u}^{3}}3a_{1u}^{1}\}$	3.54
$^{3}A_{1u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}\mathbf{23a_{1g}^{1}}33e_{u}^{4}3a_{1u}^{1}\}$	3.96
$^{1}A_{1u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}\mathbf{23a_{1g}^{1}}33e_{u}^{4}3a_{1u}^{1}\}$	3.98
$^{3}A_{2g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}\mathbf{22a_{2u}^{1}}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.13
$^{1}A_{2g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}\mathbf{22a_{2u}^{1}}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.16
$^{3}E_{g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}\mathbf{32e_{u}^{3}}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.42
$^{1}E_{g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}\mathbf{32e_{u}^{3}}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.45
$^{3}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}\mathbf{33e_{g}^{3}}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.72
$^{1}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}\mathbf{33e_{g}^{3}}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	4.74
$^{3}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}\mathbf{32e_{g}^{3}}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.16
$^{1}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}\mathbf{32e_{g}^{3}}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.18
$^{3}A_{2u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}\mathbf{11a_{2g}^{1}}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.41
$^{1}A_{2u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}\mathbf{11a_{2g}^{1}}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.43
$^{3}A_{1g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}\mathbf{12a_{1u}^{1}}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.67
$^{1}A_{1g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}\mathbf{12a_{1u}^{1}}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.69
$^{3}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}\mathbf{31e_{g}^{3}}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.88
$^{1}E_{u}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}21a_{2u}^{2}\mathbf{31e_{g}^{3}}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	5.91
$^{3}A_{2g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}\mathbf{21a_{2u}^{1}}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.01
$^{1}A_{2g}$	$\{\ldots 22a_{1g}^{2}31e_{u}^{4}\mathbf{21a_{2u}^{1}}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.03
$^{3}E_{g}$	$\{\ldots 22a_{1g}^{2}\mathbf{31e_{u}^{3}}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.37
$^{1}E_{g}$	$\{\ldots 22a_{1g}^{2}\mathbf{31e_{u}^{3}}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.39
$^{3}A_{1u}$	$\{\ldots \mathbf{22a_{1g}^{1}}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.41
$^{1}A_{1u}$	$\{\ldots \mathbf{22a_{1g}^{1}}31e_{u}^{4}21a_{2u}^{2}31e_{g}^{4}12a_{1u}^{2}11a_{2g}^{2}32e_{g}^{4}33e_{g}^{4}32e_{u}^{4}22a_{2u}^{2}23a_{1g}^{2}33e_{u}^{4}3a_{1u}^{1}\}$	6.43

Table S8. The computed VDEs, electron configurations, and final electronic states using the generalized Koopmans' theorem for the B_{80}^- (C_{2v}, $^2B_2$) tube. The bold-face indicates the orbitals from which an electron is detached.

State	Configuration	Theo. VDE ^{a}
$^1B_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 \mathbf{51b_2^0}\}$	3.85
$^3A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 \mathbf{50b_1^1} 51b_2^1\}$	4.08
$^1A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 \mathbf{50b_1^1} 51b_2^1\}$	4.11
$^3A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 \mathbf{50b_2^1} 50b_1^2 51b_2^1\}$	4.13
$^1A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 \mathbf{50b_2^1} 50b_1^2 51b_2^1\}$	4.15
$^3B_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 \mathbf{53a_1^1} 50b_2^2 50b_1^2 51b_2^1\}$	4.45
$^1B_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 \mathbf{53a_1^1} 50b_2^2 50b_1^2 51b_2^1\}$	4.47
$^3B_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 \mathbf{47a_2^1} 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.58
$^1B_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 \mathbf{47a_2^1} 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.61
$^3B_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 \mathbf{52a_1^1} 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.85
$^1B_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 \mathbf{52a_1^1} 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.87
$^3B_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 \mathbf{46a_2^1} 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.89
$^1B_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 \mathbf{46a_2^1} 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	4.92
$^3A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 \mathbf{49b_2^1} 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.28
$^1A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 \mathbf{49b_2^1} 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.31
$^3A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 \mathbf{49b_1^1} 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.36
$^1A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 48b_2^2 \mathbf{49b_1^1} 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.38
$^3A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 \mathbf{48b_2^1} 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.51
$^1A_1$	$\{...47b_1^2 51a_1^2 45a_2^2 48b_1^2 \mathbf{48b_2^1} 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.53
$^3A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 \mathbf{48b_1^1} 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.54
$^1A_2$	$\{...47b_1^2 51a_1^2 45a_2^2 \mathbf{48b_1^1} 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	5.56
$^3B_1$	$\{...47b_1^2 51a_1^2 \mathbf{45a_2^1} 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.05
$^1B_1$	$\{...47b_1^2 51a_1^2 \mathbf{45a_2^1} 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.07
$^3B_2$	$\{...47b_1^2 \mathbf{51a_1^1} 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.09
$^1B_2$	$\{...47b_1^2 \mathbf{51a_1^1} 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.11
$^3A_2$	$\{\mathbf{...47b_1^1} 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.13
$^1A_2$	$\{\mathbf{...47b_1^1} 51a_1^2 45a_2^2 48b_1^2 48b_2^2 49b_1^2 49b_2^2 46a_2^2 52a_1^2 47a_2^2 53a_1^2 50b_2^2 50b_1^2 51b_2^1\}$	6.15

Table S9. The B–B bond lengths (in Å) of neutral B_{80} optimized at the B3LYP/6-31G(d) and RI-MP2/6-31G(d) levels.

B–B bond	B3LYP/6-31G(d)	RI-MP2/6-31G(d)
Shared between two adjacent hexagons	1.665	1.716
On the side of each pentagon	1.738	1.707
Between the capping B atom and the vertex B	1.702	1.712

Table S10. The C–C bond lengths (in Å) of neutral C_{60} optimized at the B3LYP/6-31G(d) and RI-MP2/6-31G(d) levels, compared with the experimental data.

C–C bond	B3LYP/6-31G(d)	RI-MP2/6-31G(d)	Exp.[a]
Shared between two adjacent hexagons	1.385	1.408	1.391
On the side of each pentagon	1.464	1.448	1.452

[a] From ref. [13].

Table S11. The Mulliken atomic charges of I_h B_{80} buckyball calculated at the B3LYP/6-31G(d) level.

Boron atoms	Mulliken atomic charge
At the center of the hexagon (the capping atoms)	0.206
At the vertexes of the hexagon	–0.063

References

1. L. S. Wang, *Int. Rev. Phys. Chem*., 2016, **35**, 69-142.
2. X. Chen, Y. F. Zhao, Y. Y. Zhang and J. Li, *J. Comput. Chem*., 2019, **40**, 1105-1112.
3. X. Chen, Y. F. Zhao, L. S. Wang and J. Li, *Comput. Theor. Chem*., 2017, **1107**, 57-65.
4. Y. Zhao, X., Chen and J. Li, *Nano Research,* 2017, **10**, 3407-3420.
5. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, Jr., B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox,, Gaussian 16, Wallingford, CT (2016).
6. A. D. Becke, *Phys. Rev. A,* 1988, **38**, 3098-3100.
7. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785-789.
8. C. Adamo and V. Barone, *J. Chem. Phys., 1999,* **110**, 6158-6170.
9. V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern and L. A. Curtiss, *J. Comput. Chem.,* 2001, **22**, 976-984.
10. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys*., 2005, **7**, 3297-33054.
11. F. Neese, *Wiley Interdiscip. Rev*.: *Comput. Mol. Sci.,* 2012, *2*, 73-78.
12. D. Y. Zubarev and A. I. Boldyrev, *Phys. Chem. Chem. Phys*., 2008, **10**, 5207-5217.
13. E. F. Sheka, B. S. Razbirin and D. K. Nelson, *J. Phys. Chem. A,* 2011, **115**, 3480-3490.

Table S12. Cartesian coordinates of the buckyball (I_h), core-shell (C_1), sphere (D_{3d}), sphere (C_{3v}), volleyball (T_h), quasi-planar (C_s), and tube (D_{10d}) isomers of neutral B_{80} optimized at the B3LYP/6-31G(d) level.

(I_h) Buckyball			
B	-3.20740200	-2.73904400	-0.42134100
B	-2.50992200	-2.77474800	-2.01633000
B	-2.63760900	-1.43595800	-3.00741600
B	-3.46537100	-0.01236800	-2.43953300
B	-4.13615500	0.01143300	-0.91851700
B	-3.98994300	1.42863800	0.07558500
B	-3.77725700	0.91022200	1.72403900
B	-3.78799000	-0.82272700	1.74722300
B	-4.00593900	-1.38154200	0.11313700
B	-2.14214500	-3.59712300	0.64963700
B	-1.92147100	-3.06421500	2.20888000
B	-2.76441800	-1.65040300	2.77700400
B	-2.74466500	1.75287200	2.73146600
B	-1.88622800	3.14295700	2.12738400
B	-0.29593500	3.15242400	2.83718000
B	-0.16163600	1.75631100	3.84613500
B	-1.67749100	0.89027500	3.78128700
B	-1.68662100	-0.77189800	3.80329100
B	-0.18050100	-1.65246800	3.89102000
B	-0.33046000	-3.07223500	2.91810600
B	0.97579800	-3.60719300	2.02459000
B	0.73785300	-4.15539900	0.38931600
B	2.10122500	-3.63728100	-0.55460300
B	1.88623100	-3.14296000	-2.12738600
B	2.74466600	-1.75287700	-2.73146600
B	1.67748900	-0.89027600	-3.78129000
B	1.68662200	0.77189700	-3.80329700
B	0.18050100	1.65246500	-3.89102400
B	0.33046100	3.07223900	-2.91810400
B	-0.97579500	3.60719300	-2.02458700
B	-0.73785400	4.15540400	-0.38931700
B	0.78426400	4.15579800	0.28057300
B	2.14214300	3.59712600	-0.64963700
B	1.92147100	3.06422000	-2.20888200
B	2.76441700	1.65040100	-2.77700200
B	3.78798700	0.82272600	-1.74722200
B	4.00594500	1.38154300	-0.11313400
B	4.13615400	-0.01142900	0.91851700
B	3.46536900	0.01237200	2.43953200
B	2.63761400	1.43595900	3.00742000
B	1.27150200	0.91819300	3.92974600
B	1.26196800	-0.82847300	3.95283800
B	2.62276400	-1.38587100	3.04534600
B	2.47992700	-2.74928000	2.08954800
B	3.17643500	-2.76257200	0.49429800
B	3.98994200	-1.42864100	-0.07558900
B	3.77726200	-0.91022700	-1.72403900
B	-0.78426200	-4.15579200	-0.28057200
B	-1.01651000	-3.64926100	-1.92968700
B	0.29593400	-3.15242200	-2.83717900

B	0.16163600	-1.75631400	-3.84613900
B	-1.27150500	-0.91819400	-3.92975000
B	-1.26196600	0.82847000	-3.95283800
B	-2.62277100	1.38587000	-3.04534500
B	-3.17643800	2.76257200	-0.49430300
B	-2.10122100	3.63727600	0.55460300
B	1.01650900	3.64926100	1.92968700
B	2.50992700	2.77475100	2.01633100
B	3.20740400	2.73904600	0.42134600
B	-2.47993500	2.74928100	-2.08954700
B	0.19659200	-0.05229600	-3.88958500
B	-0.56620900	-3.53877200	1.29273900
B	-2.88894000	2.22824400	1.09798200
B	2.88890300	-2.22821900	-1.09797000
B	-3.26317400	-1.36214200	-1.42044700
B	-0.19659400	0.05229400	3.88961300
B	0.56620500	3.53875000	-1.29272900
B	3.26313800	1.36212800	1.42043400
B	-2.90907300	-2.16254600	1.15427700
B	-2.62933800	0.04918100	2.64749100
B	1.09226500	-2.12613600	2.86390100
B	3.24241700	-1.35857700	1.45420500
B	2.62935300	-0.04918500	-2.64750800
B	-3.24235900	1.35855100	-1.45417800
B	-0.52560200	3.57307600	1.19793100
B	2.90909100	2.16256200	-1.15428200
B	0.52560400	-3.57308800	-1.19793400
B	-1.11571500	-2.18845600	-2.80664200
B	-1.09228200	2.12616300	-2.86394000
B	1.11571900	2.18846400	2.80665300
(C_1) Core-shell			
B	2.86096100	-3.54365600	0.34239700
B	0.23796800	0.53707600	-2.57586600
B	2.52779200	-1.65737800	2.40373200
B	4.15244900	-0.94763500	0.19397100
B	3.96281700	0.57589500	0.67689200
B	2.19854700	4.13930500	-0.53779600
B	-2.67316900	-1.60422100	-3.00816500
B	1.60783800	-3.03933000	-2.46149800
B	-0.42487800	0.09340800	0.75696500
B	1.49894600	-1.16808900	3.58292400
B	0.48972000	1.50340300	0.25580100
B	-1.97531700	2.73600300	1.47212100
B	-2.99535300	1.30703600	-2.52562800
B	-2.12199600	3.99171200	0.42341800
B	1.14394200	3.43363000	-1.74293800
B	-0.78178000	0.13338400	2.39908400
B	-0.16337300	-1.27863700	3.62199000
B	-3.53495200	-0.21046000	-2.92204200
B	-1.17412200	1.40001400	-0.24769800
B	-3.22684300	2.89226100	-1.96295000
B	3.08134400	1.15033200	2.01299300
B	-0.02762900	1.63630000	3.14480800

B	1.26358900	-3.93820300	0.25983600
B	3.48564100	-2.20560000	1.15565700
B	0.01153800	-3.30355100	-2.82236300
B	-0.37699000	-2.89495100	-0.02754200
B	-3.80710800	-0.09176800	1.49972400
B	-3.57595000	-2.41406800	-0.34506600
B	-4.10125200	1.92093200	-1.01856400
B	-0.14099200	-1.26382400	-0.32216900
B	3.79708200	-2.51217000	-0.48382800
B	3.81469300	2.15591700	0.98299800
B	-1.78162300	-1.25180800	3.32125900
B	-2.59743600	-2.77236100	-1.66822600
B	-0.68536900	2.98394100	2.59391200
B	-0.74761800	-0.81237900	-1.95313500
B	1.19526500	-0.15474300	0.13098900
B	0.69946400	4.75393000	-0.86766100
B	0.70894800	2.68840600	1.60087100
B	-0.76909000	3.96444200	1.35698900
B	-3.83082400	-1.37626900	-1.64984200
B	-0.38883400	3.73753000	-1.63611100
B	-1.55093500	-0.25716700	-0.51592700
B	4.08074100	1.77825600	-0.70014500
B	1.37762400	0.95055600	-1.21781600
B	-2.11975500	-3.53940300	-0.25860400
B	-2.67857000	2.39684900	-0.06020500
B	-2.40344800	-2.44470800	2.19596100
B	-3.70366100	-1.78921100	1.16300300
B	-0.01063800	1.93878900	-1.47875500
B	-1.39102300	0.83270400	-1.95203200
B	-2.06082300	3.85881300	-1.24485000
B	2.24258300	-3.76958900	-1.08669800
B	4.05190600	-1.33485600	-1.57137900
B	0.27087500	-3.52622400	1.59733000
B	-1.50329100	-3.51554300	1.33015700
B	2.73182300	2.75873400	-1.57216600
B	-0.77191600	-2.48863100	2.43723400
B	0.97276000	-0.75949800	-1.53549600
B	2.93603600	1.21709700	-2.01679800
B	3.47432900	3.34155000	-0.06888500
B	-4.06274700	0.27648700	-1.37705100
B	-4.00190100	0.93992100	0.26179700
B	3.41994200	-0.30062000	-2.62726700
B	2.34291800	0.01468100	2.87713100
B	-0.78933700	4.69882500	-0.19889800
B	2.31903600	-1.51949000	-2.41756700
B	-1.30990300	-2.37802400	-2.89717900
B	0.70331100	0.27800400	3.48952600
B	-1.08373800	-3.63341500	-1.53482300
B	-3.32388600	-1.16757800	2.62735300
B	0.88887300	-2.44176200	2.71045200
B	-3.13652500	-0.63951300	-0.14720200
B	2.53868900	-0.39925200	1.09859600
B	4.37960500	0.31625000	-1.31201800

B	0.57752000	-3.91814100	-1.37589200
B	-2.55221800	0.28582900	2.82906200
B	1.79589600	0.13746600	-2.87527400
B	2.27081700	2.82624900	1.17642600
B	-1.75701200	1.68181200	2.83865600
(D_{3d}) Sphere			
B	-3.95837200	0.82000700	-1.47246700
B	-3.95718500	-0.92025900	-1.41405800
B	-2.86241800	-1.50780100	-2.73549400
B	-2.86376400	1.31868300	-2.83075600
B	-2.31194300	-0.12655000	-3.74082000
B	-3.95770500	1.68434700	-0.08495400
B	-2.86269800	3.12293500	0.06575200
B	-2.30997500	3.30268900	1.76387100
B	-3.95614000	0.86469600	1.45126200
B	-2.86054100	1.79179200	2.56079200
B	-3.95600200	-1.68967200	0.02825400
B	-3.95531200	-0.76904300	1.50613900
B	-2.85885200	-1.61855200	2.67516000
B	-2.85969400	-3.11394700	0.27496800
B	-2.30693700	-3.17909600	1.98125000
B	-1.90419100	-2.79460800	-2.43249900
B	-1.90274100	-3.57828800	-0.96365800
B	-0.30349300	-4.11763200	-0.67462000
B	-0.30563300	-2.85373800	-3.04349700
B	0.72626300	-3.77686600	-2.01547200
B	-1.90643700	2.62330300	-2.61422000
B	-0.30804600	2.64293000	-3.22806800
B	0.72281800	3.63388200	-2.26400200
B	-1.90600400	3.50358700	-1.20128200
B	-0.30729900	4.06289900	-0.94915400
B	-0.72849500	-0.14391000	-4.27809500
B	0.30298600	-1.47414400	-3.90310100
B	1.90184300	-0.95229100	-3.58151500
B	0.30182900	1.20935100	-3.99340100
B	1.90109300	0.71156600	-3.63737800
B	3.95837500	-0.82000600	1.47246600
B	2.86376700	-1.31868300	2.83075700
B	2.31194600	0.12655000	3.74082000
B	3.95718600	0.92026000	1.41405600
B	2.86242000	1.50780300	2.73549300
B	3.95770700	-1.68434600	0.08495100
B	3.95613900	-0.86469400	-1.45126400
B	2.86053900	-1.79178900	-2.56079200
B	2.86269900	-3.12293400	-0.06575400
B	2.30997500	-3.30268600	-1.76387300
B	1.90643900	-2.62330500	2.61422100
B	1.90600600	-3.50359000	1.20128100
B	0.30730000	-4.06290300	0.94915200
B	0.30804700	-2.64293200	3.22807000
B	-0.72282000	-3.63388700	2.26400300
B	0.72849700	0.14391100	4.27809900
B	-0.30182900	-1.20935200	3.99340300

B	-1.90109600	-0.71156700	3.63738200
B	-0.30298600	1.47414600	3.90310500
B	-1.90184600	0.95229400	3.58151900
B	3.95600000	1.68967200	-0.02825600
B	2.85969300	3.11394600	-0.27497000
B	2.30693400	3.17909300	-1.98125000
B	3.95530900	0.76904300	-1.50614000
B	2.85884900	1.61855000	-2.67515900
B	1.90419200	2.79461000	2.43249800
B	0.30563300	2.85374100	3.04349800
B	-0.72626400	3.77686800	2.01547100
B	1.90274100	3.57828700	0.96365600
B	0.30349300	4.11763100	0.67461800
B	1.26917600	3.58276700	-0.57133600
B	1.26860000	2.09202400	-2.96514100
B	1.27034000	-2.28462800	-2.81753800
B	1.27281500	-3.61281300	-0.32991400
B	-1.26917700	-3.58277000	0.57133600
B	-3.58584000	-0.00146000	0.00207000
B	-1.26860100	-2.09202700	2.96514400
B	1.27395500	-1.29655400	3.38702100
B	1.27283800	1.52202600	3.29249000
B	-1.27034100	2.28463200	2.81754000
B	-1.27281400	3.61281200	0.32991200
B	-1.27395000	1.29655200	-3.38701400
B	-1.27283700	-1.52202400	-3.29249300
B	3.58584000	0.00146100	-0.00207100
B	-3.70125000	2.51010800	1.34222200
B	-3.70276400	-0.09691100	-2.84295800
B	-3.69888800	-2.41784000	1.50744700
B	3.70276800	0.09691200	2.84295800
B	3.70124900	-2.51010600	-1.34222500
B	3.69888500	2.41783800	-1.50744800
(C_{3v}) Sphere			
B	-1.84367300	3.27099000	-2.28540500
B	-2.60108100	1.70964400	-2.79906300
B	-3.64784000	0.92723000	-1.88457700
B	-4.04163400	1.48160700	-0.25438500
B	-3.22521400	2.75607500	0.34811700
B	-2.09799400	3.69593000	-0.71248100
B	-0.10846800	3.12755800	-2.77988800
B	0.06777700	1.67789000	-3.79286700
B	-1.43268500	0.82409300	-3.80439500
B	-1.44301800	-0.82227400	-3.80147100
B	-3.65929600	-0.88929900	-1.88071500
B	-4.29148700	0.02861900	0.81183000
B	-3.73121400	0.02837700	2.34933900
B	-2.82898000	1.41958100	2.87707100
B	-2.55837300	2.73708200	1.96055400
B	-1.06995700	3.58460100	1.97262900
B	-0.72602400	4.17675000	0.36783200
B	0.79330000	4.23228100	-0.21724900
B	1.08761400	3.62175700	-1.84820100

B	1.48852100	0.84578200	-3.77870800
B	2.82431500	1.41036800	-2.75051400
B	2.65526800	2.70347000	-1.83247900
B	3.30768200	2.76051700	-0.19214600
B	2.15713900	3.69745300	0.86136700
B	1.85374500	3.20617800	2.39246500
B	0.19099600	3.13812000	2.89982200
B	-0.07939500	1.71096600	4.08376100
B	-1.47817400	0.91518400	4.07307700
B	-4.06020300	-1.43187500	-0.24831200
B	0.15165300	-3.12858500	2.91321500
B	-1.11488600	-3.56275600	1.98750900
B	-0.77870900	-4.16550800	0.38484100
B	0.73996600	-4.24174200	-0.19960700
B	2.11054100	-3.72080700	0.87655100
B	2.57753600	-1.74718400	2.93159000
B	1.45950100	-0.80550100	4.10304400
B	-0.10073100	-1.69296400	4.09083100
B	-1.48937800	-0.87970600	4.07677800
B	-2.84639400	-1.37188500	2.88292000
B	-2.59232300	-2.69660900	1.97196500
B	-2.14445000	-3.67177700	-0.69719600
B	-1.88531500	-3.25744000	-2.27192600
B	-0.14832500	-3.13866700	-2.76759900
B	1.04182600	-3.64239700	-1.83323500
B	2.62085000	-2.74414700	-1.82123500
B	3.27207600	-2.80217300	-0.18036800
B	3.97465000	-1.46131700	0.42137000
B	3.60840700	-0.87454900	2.02326700
B	1.46954100	0.80398800	4.09972300
B	2.59933600	1.72685700	2.92473000
B	3.61916300	0.83767200	2.01979700
B	3.99275900	1.41335900	0.41544800
B	4.26086300	-0.02796200	-0.64822700
B	3.79091000	-0.02833600	-2.22879600
B	2.80661900	-1.45733200	-2.74458100
B	1.47781400	-0.88054000	-3.77502800
B	0.04658700	-1.69487700	-3.78610300
B	-3.25965000	-2.71353300	0.35967900
B	-2.62259500	-1.68853200	-2.79166600
B	1.81339900	-3.21932400	2.40555400
B	2.31029600	3.93146200	-0.71029800
B	-2.25806700	3.95422200	0.99191500
B	-2.81806300	0.02531400	3.65379600
B	1.34452700	-2.41310100	3.69600500
B	2.26079400	-3.96309000	-0.69408500
B	2.89596000	-0.02577600	-3.60895100
B	-1.38329000	2.48037700	-3.65212700
B	-4.55295100	0.02699200	-0.76274300
B	-2.30759000	-3.92125300	1.00813900
B	4.53801200	-0.02610400	1.06056800
B	1.37473700	2.41126500	3.68632000
B	-1.41465100	-2.47815900	-3.64164600

B	-2.73440100	2.13785600	-1.14579400
B	-0.42845900	3.45041000	-1.12799400
B	-2.75812500	-2.10546100	-1.13548300
B	-0.47209300	-3.45069200	-1.11429300
B	0.03129100	-0.00762200	-3.45289700
B	-0.03413300	0.00814300	3.84680500
B	3.23475600	1.30337400	-1.09040900
B	3.21856600	-1.34853900	-1.08508000
(T_h) Volleyball			
B	2.28315300	3.25878900	-1.64381900
B	0.90667100	3.99810200	-2.12165800
B	-2.64253300	-2.90024400	-1.77310500
B	-0.12361400	3.72755800	2.15035900
B	-1.19780200	2.46207000	2.58001800
B	0.48238400	-4.08656200	1.26615800
B	-0.83089400	1.49781200	3.94923900
B	-2.45102100	-0.51599500	-3.50175700
B	-2.92919400	-1.22735100	-2.01690400
B	1.59284900	-2.25935900	3.30043800
B	1.64910600	-2.91352300	1.71662200
B	1.68876000	1.27719900	-3.74845800
B	3.12429700	-2.83944800	0.84567300
B	-4.14263900	-0.45342700	-1.08444000
B	3.83968800	0.75587600	-1.79635800
B	2.47718100	1.67826200	-2.27978300
B	-2.82149600	2.53667200	2.03449600
B	-3.02111500	3.42296300	0.67681200
B	-2.28315900	-3.25879000	1.64383100
B	-0.90668500	-3.99812400	2.12164500
B	2.64256300	2.90029400	1.77311600
B	1.40960300	3.49542500	2.66502500
B	0.12361700	-3.72756500	-2.15036300
B	-0.48238700	4.08651100	-1.26617300
B	0.83091600	-1.49781200	-3.94922100
B	1.19781700	-2.46209400	-2.58002100
B	2.45099400	0.51599400	3.50173500
B	-1.59291100	2.25942100	-3.30049200
B	-1.68873100	-1.27721300	3.74846700
B	-2.47716100	-1.67824700	2.27978200
B	-3.12431700	2.83943100	-0.84567600
B	4.14265800	0.45347400	1.08446200
B	-3.83965800	-0.75585600	1.79635300
B	2.82153300	-2.53675600	-2.03454900
B	1.36185900	2.72255800	-3.05673500
B	-2.02034000	-2.06550900	-3.20442800
B	-1.40961000	-3.49540800	-2.66501800
B	0.27902300	2.58647800	3.44182500
B	0.37896900	-3.24436000	2.81962000
B	-2.44775500	1.48398000	3.22872000
B	-3.56767300	0.31543900	-2.40833600
B	3.02722000	-2.06311300	2.28149900
B	2.70787400	-1.09630800	3.57314100
B	2.98846600	0.26296200	-3.10273500

B	1.80841300	-3.90330600	0.32634800
B	3.02107300	-3.42294700	-0.67679900
B	-3.67420200	-2.13003800	-0.76416800
B	-4.44665000	-1.18877100	0.34254500
B	3.48355900	2.32043000	-1.04915000
B	-1.61816200	3.71325400	1.48593600
B	-1.36185800	-2.72257400	3.05672900
B	2.02036300	2.06553300	3.20443200
B	-0.27901100	-2.58646200	-3.44179800
B	-0.37895800	3.24431600	-2.81964800
B	-1.64913600	2.91352000	-1.71664000
B	2.44780700	-1.48400200	-3.22871700
B	1.89068100	-0.27982900	-4.20079900
B	3.56760800	-0.31544400	2.40829200
B	-3.02727200	2.06317300	-2.28154600
B	-2.98842500	-0.26296600	3.10274300
B	-1.80840500	3.90323500	-0.32634700
B	3.67425000	2.13009700	0.76419400
B	2.92918100	1.22738200	2.01691400
B	-3.48353100	-2.32039600	1.04912300
B	1.61817500	-3.71330600	-1.48597400
B	0.32611100	0.19911500	-4.13869300
B	-1.17433800	0.64842800	-3.93302200
B	-0.32609600	-0.19914500	4.13873700
B	1.17436800	-0.64840800	3.93307800
B	-3.64640300	1.91345400	0.58393100
B	-4.11098500	0.40773300	0.47463000
B	3.64634100	-1.91343100	-0.58396700
B	4.11091800	-0.40771400	-0.47458000
B	4.44659900	1.18878800	-0.34252600
B	-1.12107600	-3.97397600	0.49914600
B	-1.28530000	-3.80961700	-1.06345500
B	1.12104200	3.97396700	-0.49914900
B	1.28530700	3.80959400	1.06344900
B	-2.70785000	1.09629400	-3.57309800
B	-1.89064700	0.27981200	4.20084300
(C_s) Quasi-planar			
B	4.51533400	-3.24166200	0.44124000
B	0.39731800	-5.82465000	-0.14773500
B	3.17114000	-2.46595500	-0.56818000
B	0.40179800	-4.23026400	-0.75710400
B	-2.47357700	-4.21391700	-0.39275300
B	3.30192000	-0.82820000	-0.85075100
B	-1.03170100	-3.35338800	-0.80895900
B	3.17119800	2.46592100	-0.56823500
B	0.41923000	-0.84654700	-1.18043700
B	-1.04673200	-5.03674500	-0.39212000
B	3.27631900	-4.20116900	-0.26284600
B	4.55403200	-1.63100100	0.09027600
B	3.30196000	0.82815700	-0.85082200
B	0.40186500	4.23026500	-0.75715700
B	1.80790000	-4.95230100	-0.17987400
B	-2.51774200	0.81442300	-0.91299600

B	-2.46777400	-2.51469400	-0.80015700
B	-1.02738700	1.71735400	-1.06048500
B	4.55408500	1.63095100	0.09021500
B	-1.03165500	3.35339500	-0.80897600
B	-3.92390600	-1.66307800	-0.61720700
B	-3.92391600	1.66314000	-0.61726600
B	-3.93567600	-3.38450500	-0.31976700
B	-2.46776200	2.51473600	-0.80025500
B	1.82294900	-1.68138900	-0.98786100
B	-0.99163600	0.00001900	-1.06557400
B	-1.02739900	-1.71733800	-1.06046400
B	0.41923500	0.84657600	-1.18048700
B	-5.24984500	2.49377300	0.08994500
B	-5.32590200	0.84909200	-0.32383200
B	-5.32588900	-0.84899900	-0.32379400
B	-5.22886500	-4.15820700	0.46556600
B	-2.45728700	-5.80433300	0.18586700
B	-1.04841800	-6.61898600	0.43424400
B	6.06365500	-0.81161800	0.24118600
B	6.06366000	0.81154000	0.24123100
B	6.05590900	2.47717300	0.18021700
B	1.80798100	4.95232500	-0.17994900
B	0.39738700	5.82462900	-0.14772500
B	-1.04666000	5.03677300	-0.39217900
B	-2.47350100	4.21392900	-0.39269900
B	-3.93562300	3.38455700	-0.31974400
B	3.27638900	4.20116600	-0.26288200
B	4.51538100	3.24161400	0.44113300
B	-5.24992600	-2.49372600	0.08980800
B	-3.87448800	-5.02278000	0.26714200
B	6.05584800	-2.47724600	0.18023600
B	7.47241700	1.65026100	0.83210700
B	7.46633100	-0.00005400	0.67769200
B	7.47238000	-1.65037100	0.83208100
B	-6.65550400	1.65284500	0.38920900
B	-6.60942700	0.00004400	0.37782300
B	-6.65552600	-1.65275800	0.38918100
B	-6.58253400	-3.34271000	0.90539400
B	-2.51773800	-0.81438300	-0.91302100
B	1.83642300	-3.37493900	-0.83024700
B	1.82299200	1.68137000	-0.98791300
B	1.83649700	3.37493900	-0.83031700
B	1.79955000	6.60446300	0.53142200
B	3.21203500	5.76175100	0.44593400
B	4.59345400	4.93876700	0.57504800
B	6.00680600	4.12290700	0.75370200
B	7.26778700	3.20410300	1.05673500
B	-7.74929300	2.40062600	1.39495500
B	-7.90515000	0.82818100	1.24647800
B	-7.90516500	-0.82811700	1.24645800
B	-7.74937700	-2.40057700	1.39482000
B	7.26775900	-3.20421900	1.05668200
B	6.00675800	-4.12299900	0.75368800

B	4.59337900	-4.93882100	0.57507700
B	3.21194500	-5.76177600	0.44598100
B	1.79945100	-6.60448200	0.53137600
B	0.37375300	-7.23111000	0.74508500
B	0.37385400	7.23109000	0.74512000
B	-1.04832700	6.61900800	0.43424200
B	-2.45719800	5.80436000	0.18588400
B	-3.87438900	5.02279800	0.26721100
B	-5.22878200	4.15825200	0.46566200
B	-6.58243800	3.34276100	0.90554500
B	4.43804800	-0.00002000	0.25387500
(D_{10d}) Tube			
B	-10.17195600	-0.91989800	0.75726000
B	-0.68136400	-10.17306400	0.75654300
B	-9.88721100	-2.49588600	0.75536900
B	-9.38973900	-4.01787300	0.75759200
B	-8.63183000	-5.42867900	0.75582300
B	-7.68828800	-6.72238700	0.75809100
B	-6.53151200	-7.82994500	0.75628300
B	-5.23436800	-8.76876400	0.75847200
B	-3.79196800	-9.46471400	0.75652100
B	-2.26824500	-9.95691100	0.75857600
B	10.17450100	-0.68157200	0.75678600
B	0.91988400	-10.17049900	0.75849300
B	9.95821700	-2.26847100	0.75865700
B	9.46616100	-3.79220900	0.75648800
B	8.77002700	-5.23455700	0.75838400
B	7.83094900	-6.53147700	0.75634600
B	6.72301400	-7.68794200	0.75825900
B	5.42901500	-8.63105900	0.75633200
B	4.01798100	-9.38861200	0.75829500
B	2.49591700	-9.88587800	0.75641300
B	-10.17455100	0.68132100	0.75522300
B	-0.91991600	10.17064900	0.76015100
B	-9.95823200	2.26815900	0.75733700
B	-9.46588700	3.79180600	0.75552200
B	-8.76972000	5.23409600	0.75783700
B	-7.83071700	6.53108700	0.75619700
B	-6.72286100	7.68759900	0.75862200
B	-5.42899900	8.63092500	0.75703900
B	-4.01803600	9.38860500	0.75946900
B	-2.49594300	9.88576400	0.75778900
B	10.17168200	0.91965000	0.75907400
B	0.68130500	10.17336400	0.75826200
B	9.88675500	2.49566900	0.75722000
B	9.38945300	4.01771600	0.75959000
B	8.63160300	5.42862200	0.75773900
B	7.68814400	6.72237900	0.76013300
B	6.53144200	7.83011600	0.75823000
B	5.23437600	8.76900600	0.76048000
B	3.79185600	9.46484100	0.75845600
B	2.26823700	9.95733100	0.76049400
B	-10.05229800	-1.71253100	-0.75815400

B	0.11917800	-10.21144300	-0.75895600
B	-9.67576200	-3.26919100	-0.76005100
B	-9.03119300	-4.73496200	-0.75777200
B	-8.19200000	-6.09903600	-0.75956400
B	-7.12596400	-7.29381400	-0.75729300
B	-5.90627800	-8.33174500	-0.75912100
B	-4.52313400	-9.13850700	-0.75697500
B	-3.04240900	-9.74874100	-0.75890500
B	-1.47762500	-10.08851500	-0.75691300
B	10.21227400	0.11921900	-0.75860400
B	1.71235800	-10.05106900	-0.75704700
B	10.08933700	-1.47757300	-0.75671700
B	9.74960000	-3.04236700	-0.75896500
B	9.13916400	-4.52297500	-0.75702100
B	8.33226700	-5.90605600	-0.75915700
B	7.29409500	-7.12549200	-0.75719100
B	6.09907400	-8.19128600	-0.75921300
B	4.73479100	-9.03008300	-0.75719400
B	3.26904100	-9.67473600	-0.75912800
B	-10.21224200	-0.11928900	-0.76028100
B	-1.71228900	10.05157400	-0.75544800
B	-10.08925600	1.47753000	-0.75818500
B	-9.74905200	3.04222200	-0.76009700
B	-9.13871600	4.52290800	-0.75779300
B	-8.33166500	5.90588700	-0.75951300
B	-7.29371000	7.12555000	-0.75706000
B	-6.09879100	8.19142800	-0.75869700
B	-4.73472900	9.03061600	-0.75620000
B	-3.26894200	9.67511100	-0.75789900
B	10.05195300	1.71241000	-0.75632400
B	-0.11910200	10.21175600	-0.75734800
B	9.67534600	3.26903100	-0.75811500
B	9.03078200	4.73479500	-0.75581100
B	8.19169200	6.09891400	-0.75760000
B	7.12569000	7.29372100	-0.75526600
B	5.90612300	8.33173700	-0.75720700
B	4.52311100	9.13870800	-0.75494700
B	3.04235600	9.74879700	-0.75709400
B	1.47774200	10.08918900	-0.75501900