

Supporting Information

Discovering SnB_7^- : a half-sandwich structure with double aromaticity and pathways to molecular machines

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Table S1. Cartesian coordinates of the global minimum structure of the SnB_n^- ($n=5-14$) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP Level.

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Table S4. The X and Y coordinate positions of the B, Sn and Bq atoms in the NICS scanning curves of SnB_7^- , along with the Z coordinates in different reference curves (-1.0 Å, 0.5 Å, and 1.0 Å)

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Figure S1. The global minimum structures and three low-lying isomers of SnB_n^- ($n=5-9$) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level, with point group symmetries and electronic states. Relative energies are calculated at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level in parentheses and DLPNO-CCSD(T)/def2-TZVP level in square brackets.

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Figure S2. The global minimum structures and three low-lying isomers of SnB_n^- ($n=10-14$) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level, with point group symmetries

and electronic states. Relative energies are calculated at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level in parentheses and DLPNO-CCSD(T)/def2-TZVP level in square brackets.

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Figure S3. a) At least three coexisting isomers of B_7^- have been confirmed in the experiment, and b) the experimental (black line) and simulated (colored lines) photoelectron spectra for different isomers.

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Figure S4. Infrared spectra of the global minimum structure, local minimum structure, and transition state structure of SnB_7^- .

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Table S1. Cartesian coordinates of the global minimum structure of the SnB_n^- ($n=5-14$) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level.

Clusters	Atoms	X-axis	Y-axis	Z-axis
SnB_5^-	B	-0.62362100	-1.15462700	0.00000000
	B	1.05748400	-0.80419800	0.00000000
	B	-0.02211700	-3.84555900	0.00000000
	B	0.63551400	-2.33385700	0.00000000
	B	-1.04726100	-2.67257800	0.00000000
	Sn	0.00000000	1.08108200	0.00000000
SnB_6^-	B	0.00000000	1.03401300	0.00000000
	B	1.66876200	1.39732900	0.00000000
	B	2.02490800	2.95611800	0.00000000
	B	0.37892000	2.59230900	0.00000000
	B	1.01915600	4.09380000	0.00000000
	B	1.18936100	-0.13617200	0.00000000
SnB_7^-	Sn	-0.62811100	-1.19374000	0.00000000
	B	0.00000000	1.61090800	-1.12611200
	B	-1.39508700	0.80545400	-1.12611200
	B	1.39508700	-0.80545400	-1.12611200
	B	1.39508700	0.80545400	-1.12611200
	B	0.00000000	0.00000000	-1.55321200
	B	0.00000000	-1.61090800	-1.12611200
SnB_8^-	B	-1.39508700	-0.80545400	-1.12611200
	Sn	0.00000000	0.00000000	0.83098800
	B	-1.11668700	-0.38506400	1.66440300
	B	-1.48228300	-0.28711900	0.00000000
	B	-1.11668700	1.09795300	1.12629600
	B	-1.11668700	1.09795300	-1.12629600
	B	-1.03231600	-1.70230800	0.79075000
	B	-1.03231600	-1.70230800	-0.79075000
SnB_9^-	B	-0.78549100	2.21739600	0.00000000
	B	-1.11668700	-0.38506400	-1.66440300
	Sn	0.87991500	0.00485600	0.00000000
	B	2.75227700	0.21280500	0.00000000
	B	0.56387100	2.86145600	0.00000000
SnB_{10}^-	B	1.57161600	1.37179800	0.00000000
	B	-0.91450800	2.26478700	0.00000000
	B	-1.61250600	0.89314500	0.00000000
	B			

	B	3.15892000	1.74284500	0.00000000
	B	0.00000000	0.82728500	0.00000000
	B	1.26805800	-0.28945600	0.00000000
	B	2.12807800	2.94260800	0.00000000
	Sn	-0.89158100	-1.28272700	0.00000000
	B	-2.86734500	-1.56402900	-0.46383200
	B	-0.20688500	1.48968800	0.36375800
	B	-3.16437900	0.00004100	-0.39503900
	B	-0.41739800	-0.00003200	1.02840300
	B	-1.51811000	2.27454000	-0.17413400
SnB ₁₀ ⁻	B	-1.76552100	0.83712800	0.54789300
	B	-1.76559800	-0.83704000	0.54779800
	B	-0.20700000	-1.48974600	0.36379900
	B	-2.86723300	1.56409900	-0.46381100
	B	-1.51824500	-2.27451500	-0.17413100
	Sn	1.62977100	-0.00001300	-0.11807000
	B	0.40130700	1.68783300	0.66018700
	B	-2.26257600	0.00000400	-0.38386800
	B	-0.81858000	-0.85324400	-0.12939000
	B	-2.37872200	-1.71278100	0.01398100
	B	-0.81854000	0.85325900	-0.12940900
SnB ₁₁ ⁻	B	-1.00038400	-2.34199200	0.52375600
	B	-3.68403900	-0.76968300	-0.23341900
	B	0.40127400	-1.68781100	0.66019900
	B	-1.00035700	2.34200900	0.52374500
	B	-2.37868100	1.71276400	0.01399600
	B	-3.68402600	0.76971600	-0.23340000
	B	2.45256400	-0.84257300	0.33638800
	B	1.00338000	0.00000100	0.11125000
	B	3.88397800	1.57830400	-0.02438700
	B	2.45256300	0.84257200	0.33638400
	B	1.05805100	1.72000200	-0.19478300
	B	-0.37596000	-0.87563300	-0.20883700
SnB ₁₂ ⁻	B	1.05805100	-1.72000100	-0.19477800
	B	2.53896900	2.35850800	-0.21064900
	B	4.09784000	-0.00000100	0.14528500
	B	2.53896800	-2.35850800	-0.21065300
	B	-0.37596100	0.87563500	-0.20883500
	B	3.88397700	-1.57830500	-0.02438900
	Sn	-2.42164200	0.00000000	0.03480000

	B	0.46853011	4.07606484	0.00000000
	B	0.11210460	2.50344237	0.00000000
	B	-0.75603795	0.29593587	1.56726854
	B	-0.75603795	0.29593587	-1.56726854
	B	0.28680171	3.34587403	-1.40716417
	B	-1.80115060	-1.81051952	0.00000000
	B	-1.42480031	-0.18505097	0.00000000
SnB ₁₃ ⁻	B	-0.20638888	0.92156306	0.00000000
	B	-0.13816240	1.85541942	1.59625172
	B	-0.13816240	1.85541942	-1.59625172
	B	0.28680171	3.34587403	1.40716417
	B	-1.41148269	-1.16254298	-1.39458967
	B	-1.41148269	-1.16254298	1.39458967
	Sn	0.68894677	-1.41748725	0.00000000
	B	-0.36949500	2.03553900	0.84213300
	B	-0.19898200	0.54970400	0.00000000
	B	-0.10470800	3.46093300	0.00000000
	B	-0.36949500	2.03553900	-0.84213300
	B	-0.08405300	-0.80519100	-0.86442600
	B	0.25354100	4.81656500	0.78230400
	B	0.07742300	2.04700100	-2.40964900
SnB ₁₄ ⁻	B	-0.08413900	0.61248000	1.76044900
	B	0.07742300	2.04700100	2.40964900
	B	-0.08405300	-0.80519100	0.86442600
	B	-0.08413900	0.61248000	-1.76044900
	B	0.25354100	4.81656500	-0.78230400
	B	0.09619300	3.52885000	1.74778600
	B	0.09619300	3.52885000	-1.74778600
	Sn	0.05247500	-2.84811300	0.00000000

Table S2. Relative Boltzmann distribution populations of several low-lying isomers of SnB_n^- ($n=8, 11, 14$) at 298.15 K.

isomers	ΔE (kcal/mol)	percentage of populations
SnB_8^- -a	0.000	61.43%
SnB_8^- -b	0.276	38.57%
SnB_8^- -c	8.654	0.00%
SnB_8^- -d	14.744	0.00%
isomers	ΔE (kcal/mol)	percentage of populations
SnB_{11}^- -a	0.000	65.20%
SnB_{11}^- -b	0.373	34.73%
SnB_{11}^- -c	4.277	0.05%
SnB_{11}^- -d	4.700	0.02%
isomers	ΔE (kcal/mol)	percentage of populations
SnB_{14}^- -a	0.000	89.72%
SnB_{14}^- -b	1.668	5.38%
SnB_{14}^- -c	1.722	4.90%
SnB_{14}^- -d	5.857	0.00%

Table S3. The X and Y coordinate positions of the B and Bq atoms in the NICS scanning curves of B_7^- , along with the Z coordinates in different reference curves (-1.0 Å, 0.5 Å, and 1.0 Å)

Atoms	B_7^- (C_{6v} , 3A_1)				
	X	Y	Z (-1.0 Å)	Z (0.5 Å)	Z (1.0 Å)
B	0.000000	1.605000	0.000000	0.000000	0.000000
B	1.390000	0.802000	0.000000	0.000000	0.000000
B	1.390000	-0.802000	0.000000	0.000000	0.000000
B	0.000000	-1.605000	0.000000	0.000000	0.000000
B	-1.390000	0.802000	0.000000	0.000000	0.000000
B	0.000000	0.000000	-0.299000	-0.299000	-0.299000
B	-1.390000	-0.802000	0.000000	0.000000	0.000000
Bq	-5.075377	0.000000	-1.000000	0.500000	1.000000
Bq	-4.974874	0.000000	-1.000000	0.500000	1.000000
Bq	-4.874372	0.000000	-1.000000	0.500000	1.000000
Bq	-4.773869	0.000000	-1.000000	0.500000	1.000000
Bq	-4.673367	0.000000	-1.000000	0.500000	1.000000
Bq	-4.572864	0.000000	-1.000000	0.500000	1.000000
Bq	-4.472362	0.000000	-1.000000	0.500000	1.000000
Bq	-4.371859	0.000000	-1.000000	0.500000	1.000000
Bq	-4.271357	0.000000	-1.000000	0.500000	1.000000
Bq	-4.170854	0.000000	-1.000000	0.500000	1.000000
Bq	-4.070352	0.000000	-1.000000	0.500000	1.000000
Bq	-3.969849	0.000000	-1.000000	0.500000	1.000000
Bq	-3.869347	0.000000	-1.000000	0.500000	1.000000
Bq	-3.768844	0.000000	-1.000000	0.500000	1.000000
Bq	-3.668342	0.000000	-1.000000	0.500000	1.000000
Bq	-3.567839	0.000000	-1.000000	0.500000	1.000000
Bq	-3.467337	0.000000	-1.000000	0.500000	1.000000
Bq	-3.366834	0.000000	-1.000000	0.500000	1.000000
Bq	-3.266332	0.000000	-1.000000	0.500000	1.000000
Bq	-3.165829	0.000000	-1.000000	0.500000	1.000000
Bq	-3.065327	0.000000	-1.000000	0.500000	1.000000
Bq	-2.964824	0.000000	-1.000000	0.500000	1.000000
Bq	-2.864322	0.000000	-1.000000	0.500000	1.000000
Bq	-2.763819	0.000000	-1.000000	0.500000	1.000000
Bq	-2.663317	0.000000	-1.000000	0.500000	1.000000
Bq	-2.562814	0.000000	-1.000000	0.500000	1.000000
Bq	-2.462312	0.000000	-1.000000	0.500000	1.000000
Bq	-2.361809	0.000000	-1.000000	0.500000	1.000000
Bq	-2.261307	0.000000	-1.000000	0.500000	1.000000
Bq	-2.160804	0.000000	-1.000000	0.500000	1.000000
Bq	-2.060302	0.000000	-1.000000	0.500000	1.000000

Bq	-1.959799	0.000000	-1.000000	0.500000	1.000000
Bq	-1.859296	0.000000	-1.000000	0.500000	1.000000
Bq	-1.758794	0.000000	-1.000000	0.500000	1.000000
Bq	-1.658291	0.000000	-1.000000	0.500000	1.000000
Bq	-1.557789	0.000000	-1.000000	0.500000	1.000000
Bq	-1.457286	0.000000	-1.000000	0.500000	1.000000
Bq	-1.356784	0.000000	-1.000000	0.500000	1.000000
Bq	-1.256281	0.000000	-1.000000	0.500000	1.000000
Bq	-1.155779	0.000000	-1.000000	0.500000	1.000000
Bq	-1.055276	0.000000	-1.000000	0.500000	1.000000
Bq	-0.954774	0.000000	-1.000000	0.500000	1.000000
Bq	-0.854271	0.000000	-1.000000	0.500000	1.000000
Bq	-0.753769	0.000000	-1.000000	0.500000	1.000000
Bq	-0.653266	0.000000	-1.000000	0.500000	1.000000
Bq	-0.552764	0.000000	-1.000000	0.500000	1.000000
Bq	-0.452261	0.000000	-1.000000	0.500000	1.000000
Bq	-0.351759	0.000000	-1.000000	0.500000	1.000000
Bq	-0.251256	0.000000	-1.000000	0.500000	1.000000
Bq	-0.150754	0.000000	-1.000000	0.500000	1.000000
Bq	-0.050251	0.000000	-1.000000	0.500000	1.000000
Bq	0.050251	0.000000	-1.000000	0.500000	1.000000
Bq	0.150754	0.000000	-1.000000	0.500000	1.000000
Bq	0.251256	0.000000	-1.000000	0.500000	1.000000
Bq	0.351759	0.000000	-1.000000	0.500000	1.000000
Bq	0.452261	0.000000	-1.000000	0.500000	1.000000
Bq	0.552764	0.000000	-1.000000	0.500000	1.000000
Bq	0.653266	0.000000	-1.000000	0.500000	1.000000
Bq	0.753769	0.000000	-1.000000	0.500000	1.000000
Bq	0.854271	0.000000	-1.000000	0.500000	1.000000
Bq	0.954774	0.000000	-1.000000	0.500000	1.000000
Bq	1.055276	0.000000	-1.000000	0.500000	1.000000
Bq	1.155779	0.000000	-1.000000	0.500000	1.000000
Bq	1.256281	0.000000	-1.000000	0.500000	1.000000
Bq	1.356784	0.000000	-1.000000	0.500000	1.000000
Bq	1.457286	0.000000	-1.000000	0.500000	1.000000
Bq	1.557789	0.000000	-1.000000	0.500000	1.000000
Bq	1.658291	0.000000	-1.000000	0.500000	1.000000
Bq	1.758794	0.000000	-1.000000	0.500000	1.000000
Bq	1.859296	0.000000	-1.000000	0.500000	1.000000
Bq	1.959799	0.000000	-1.000000	0.500000	1.000000
Bq	2.060302	0.000000	-1.000000	0.500000	1.000000
Bq	2.160804	0.000000	-1.000000	0.500000	1.000000
Bq	2.261307	0.000000	-1.000000	0.500000	1.000000
Bq	2.361809	0.000000	-1.000000	0.500000	1.000000

Bq	2.462312	0.000000	-1.000000	0.500000	1.000000
Bq	2.562814	0.000000	-1.000000	0.500000	1.000000
Bq	2.663317	0.000000	-1.000000	0.500000	1.000000
Bq	2.763819	0.000000	-1.000000	0.500000	1.000000
Bq	2.864322	0.000000	-1.000000	0.500000	1.000000
Bq	2.964824	0.000000	-1.000000	0.500000	1.000000
Bq	3.065327	0.000000	-1.000000	0.500000	1.000000
Bq	3.165829	0.000000	-1.000000	0.500000	1.000000
Bq	3.266332	0.000000	-1.000000	0.500000	1.000000
Bq	3.366834	0.000000	-1.000000	0.500000	1.000000
Bq	3.467337	0.000000	-1.000000	0.500000	1.000000
Bq	3.567839	0.000000	-1.000000	0.500000	1.000000
Bq	3.668342	0.000000	-1.000000	0.500000	1.000000
Bq	3.768844	0.000000	-1.000000	0.500000	1.000000
Bq	3.869347	0.000000	-1.000000	0.500000	1.000000
Bq	3.969849	0.000000	-1.000000	0.500000	1.000000
Bq	4.070352	0.000000	-1.000000	0.500000	1.000000
Bq	4.170854	0.000000	-1.000000	0.500000	1.000000
Bq	4.271357	0.000000	-1.000000	0.500000	1.000000
Bq	4.371859	0.000000	-1.000000	0.500000	1.000000
Bq	4.472362	0.000000	-1.000000	0.500000	1.000000
Bq	4.572864	0.000000	-1.000000	0.500000	1.000000
Bq	4.673367	0.000000	-1.000000	0.500000	1.000000
Bq	4.773869	0.000000	-1.000000	0.500000	1.000000
Bq	4.874372	0.000000	-1.000000	0.500000	1.000000
Bq	4.974874	0.000000	-1.000000	0.500000	1.000000
Bq	5.075377	0.000000	-1.000000	0.500000	1.000000

Table S4. The X and Y coordinate positions of the B, Sn and Bq atoms in the NICS scanning curves of SnB_7^- , along with the Z coordinates in different reference curves (-1.0 Å, 0.5 Å, and 1.0 Å)

SnB_7^- (C_{6v} , 1A)					
Atoms	X	Y	Z (-1.0 Å)	Z (0.5 Å)	Z (1.0 Å)
B	0.000000	1.605000	0.000000	0.000000	0.000000
B	1.390000	0.802000	0.000000	0.000000	0.000000
B	1.390000	-0.802000	0.000000	0.000000	0.000000
B	0.000000	-1.605000	0.000000	0.000000	0.000000
B	-1.390000	0.802000	0.000000	0.000000	0.000000
B	0.000000	0.000000	-0.299000	-0.299000	-0.299000
B	-1.390000	-0.802000	0.000000	0.000000	0.000000
Sn	0.000000	0.000000	1.957000	1.957000	1.957000
Bq	-5.075377	0.000000	-1.000000	0.500000	1.000000
Bq	-4.974874	0.000000	-1.000000	0.500000	1.000000
Bq	-4.874372	0.000000	-1.000000	0.500000	1.000000
Bq	-4.773869	0.000000	-1.000000	0.500000	1.000000
Bq	-4.673367	0.000000	-1.000000	0.500000	1.000000
Bq	-4.572864	0.000000	-1.000000	0.500000	1.000000
Bq	-4.472362	0.000000	-1.000000	0.500000	1.000000
Bq	-4.371859	0.000000	-1.000000	0.500000	1.000000
Bq	-4.271357	0.000000	-1.000000	0.500000	1.000000
Bq	-4.170854	0.000000	-1.000000	0.500000	1.000000
Bq	-4.070352	0.000000	-1.000000	0.500000	1.000000
Bq	-3.969849	0.000000	-1.000000	0.500000	1.000000
Bq	-3.869347	0.000000	-1.000000	0.500000	1.000000
Bq	-3.768844	0.000000	-1.000000	0.500000	1.000000
Bq	-3.668342	0.000000	-1.000000	0.500000	1.000000
Bq	-3.567839	0.000000	-1.000000	0.500000	1.000000
Bq	-3.467337	0.000000	-1.000000	0.500000	1.000000
Bq	-3.366834	0.000000	-1.000000	0.500000	1.000000
Bq	-3.266332	0.000000	-1.000000	0.500000	1.000000
Bq	-3.165829	0.000000	-1.000000	0.500000	1.000000
Bq	-3.065327	0.000000	-1.000000	0.500000	1.000000
Bq	-2.964824	0.000000	-1.000000	0.500000	1.000000
Bq	-2.864322	0.000000	-1.000000	0.500000	1.000000
Bq	-2.763819	0.000000	-1.000000	0.500000	1.000000
Bq	-2.663317	0.000000	-1.000000	0.500000	1.000000
Bq	-2.562814	0.000000	-1.000000	0.500000	1.000000
Bq	-2.462312	0.000000	-1.000000	0.500000	1.000000
Bq	-2.361809	0.000000	-1.000000	0.500000	1.000000
Bq	-2.261307	0.000000	-1.000000	0.500000	1.000000

Bq	-2.160804	0.000000	-1.000000	0.500000	1.000000
Bq	-2.060302	0.000000	-1.000000	0.500000	1.000000
Bq	-1.959799	0.000000	-1.000000	0.500000	1.000000
Bq	-1.859296	0.000000	-1.000000	0.500000	1.000000
Bq	-1.758794	0.000000	-1.000000	0.500000	1.000000
Bq	-1.658291	0.000000	-1.000000	0.500000	1.000000
Bq	-1.557789	0.000000	-1.000000	0.500000	1.000000
Bq	-1.457286	0.000000	-1.000000	0.500000	1.000000
Bq	-1.356784	0.000000	-1.000000	0.500000	1.000000
Bq	-1.256281	0.000000	-1.000000	0.500000	1.000000
Bq	-1.155779	0.000000	-1.000000	0.500000	1.000000
Bq	-1.055276	0.000000	-1.000000	0.500000	1.000000
Bq	-0.954774	0.000000	-1.000000	0.500000	1.000000
Bq	-0.854271	0.000000	-1.000000	0.500000	1.000000
Bq	-0.753769	0.000000	-1.000000	0.500000	1.000000
Bq	-0.653266	0.000000	-1.000000	0.500000	1.000000
Bq	-0.552764	0.000000	-1.000000	0.500000	1.000000
Bq	-0.452261	0.000000	-1.000000	0.500000	1.000000
Bq	-0.351759	0.000000	-1.000000	0.500000	1.000000
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Bq	0.050251	0.000000	-1.000000	0.500000	1.000000
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Bq	0.653266	0.000000	-1.000000	0.500000	1.000000
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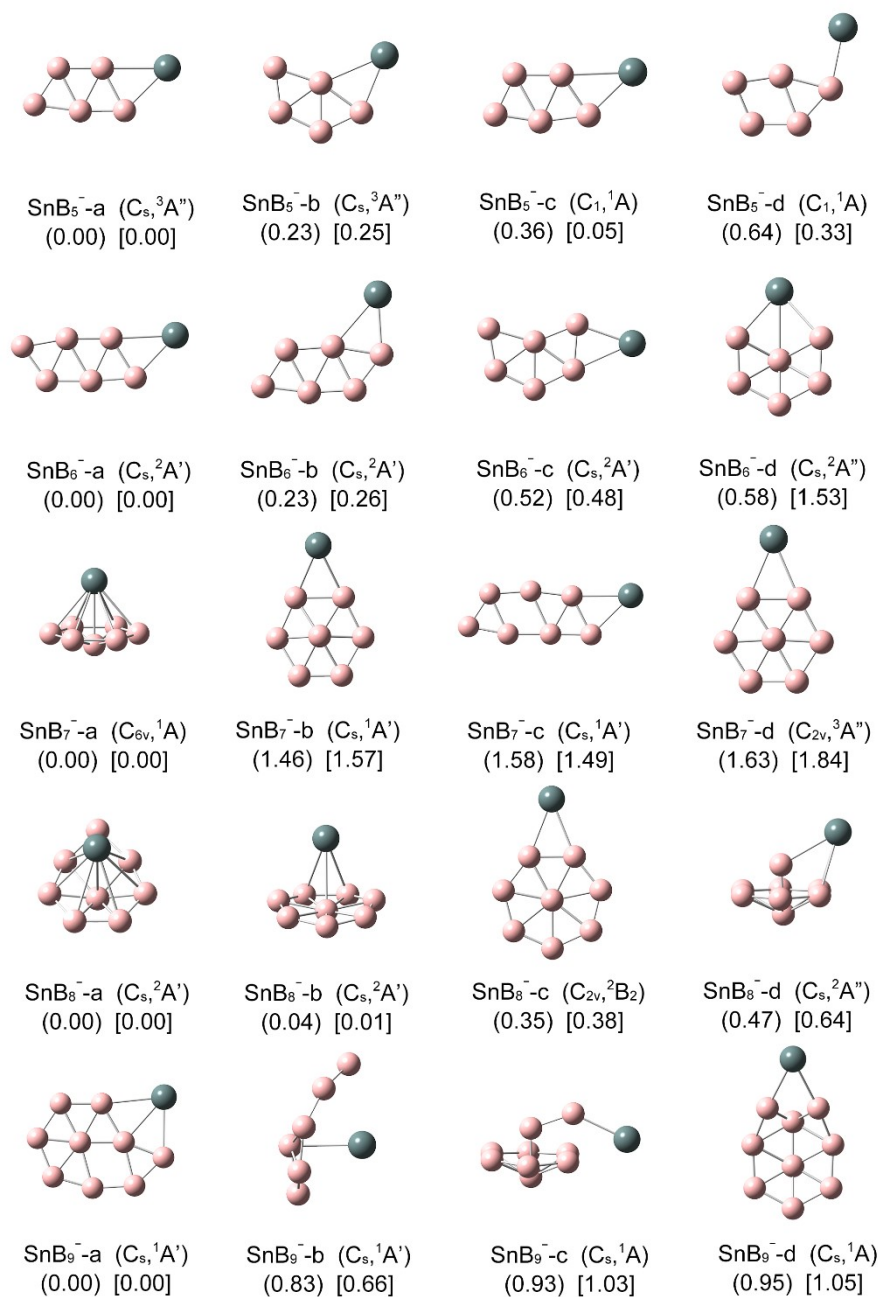


Figure S1. The global minimum structures and three low-lying isomers of SnB_n⁻ (n=5-9) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level, with point group symmetries and electronic states. Relative energies are calculated at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level in parentheses and DLPNO-CCSD(T)/def2-TZVP level in square brackets.

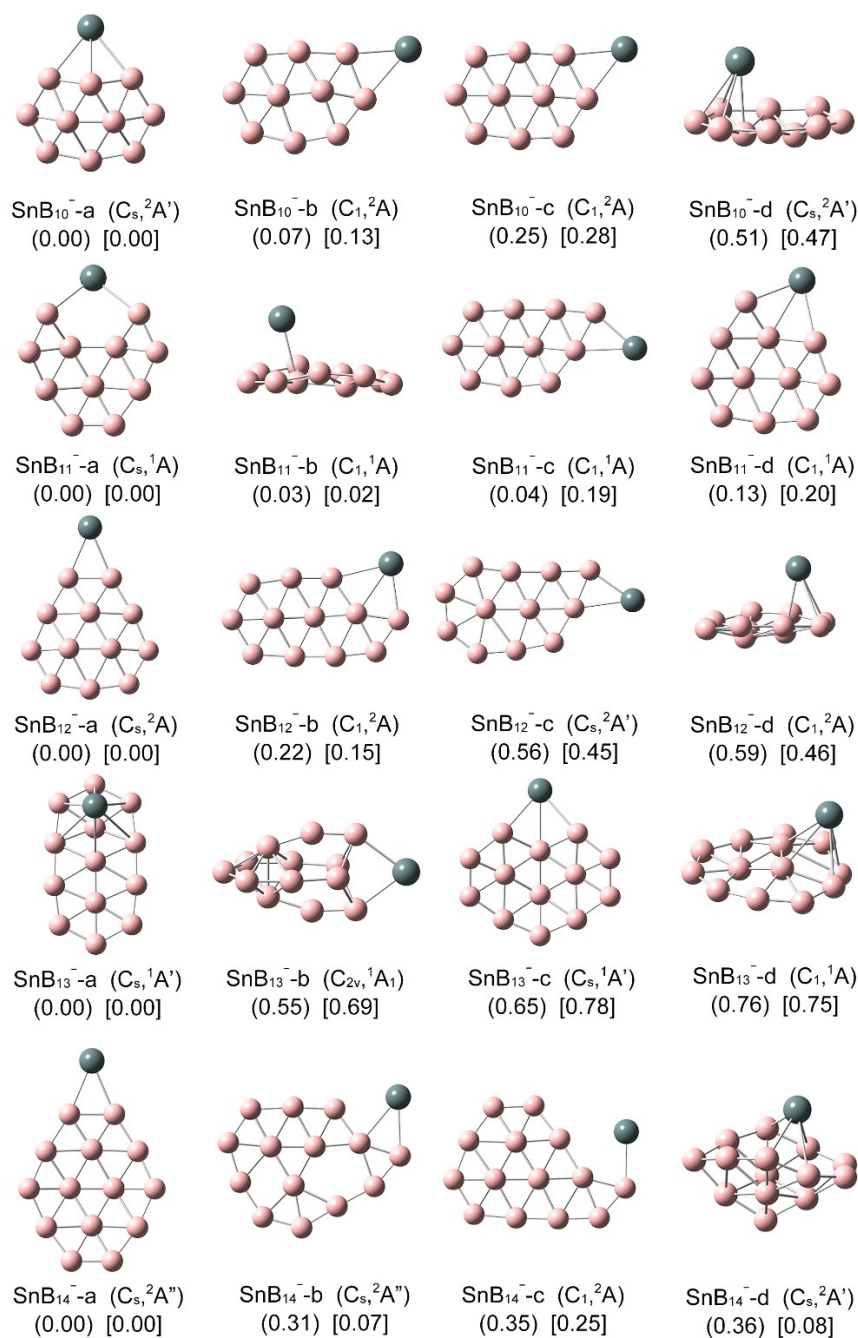


Figure S2. The global minimum structures and three low-lying isomers of SnB_n⁻ (n=10-14) optimized at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level, with point group symmetries and electronic states. Relative energies are calculated at PBE0/B/aug-cc-pVTZ//Sn/aug-cc-pVTZ-PP level in parentheses and DLPNO-CCSD(T)/def2-TZVP level in square brackets.

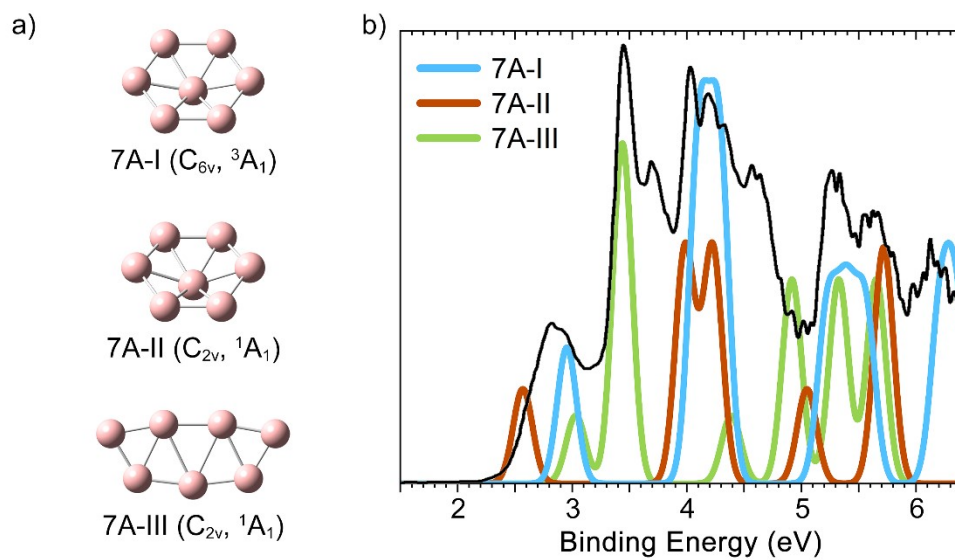


Figure S3. a) At least three coexisting isomers of B_7^- have been confirmed in the experiment, and b) the experimental (black line) and simulated (colored lines) photoelectron spectra for different isomers.

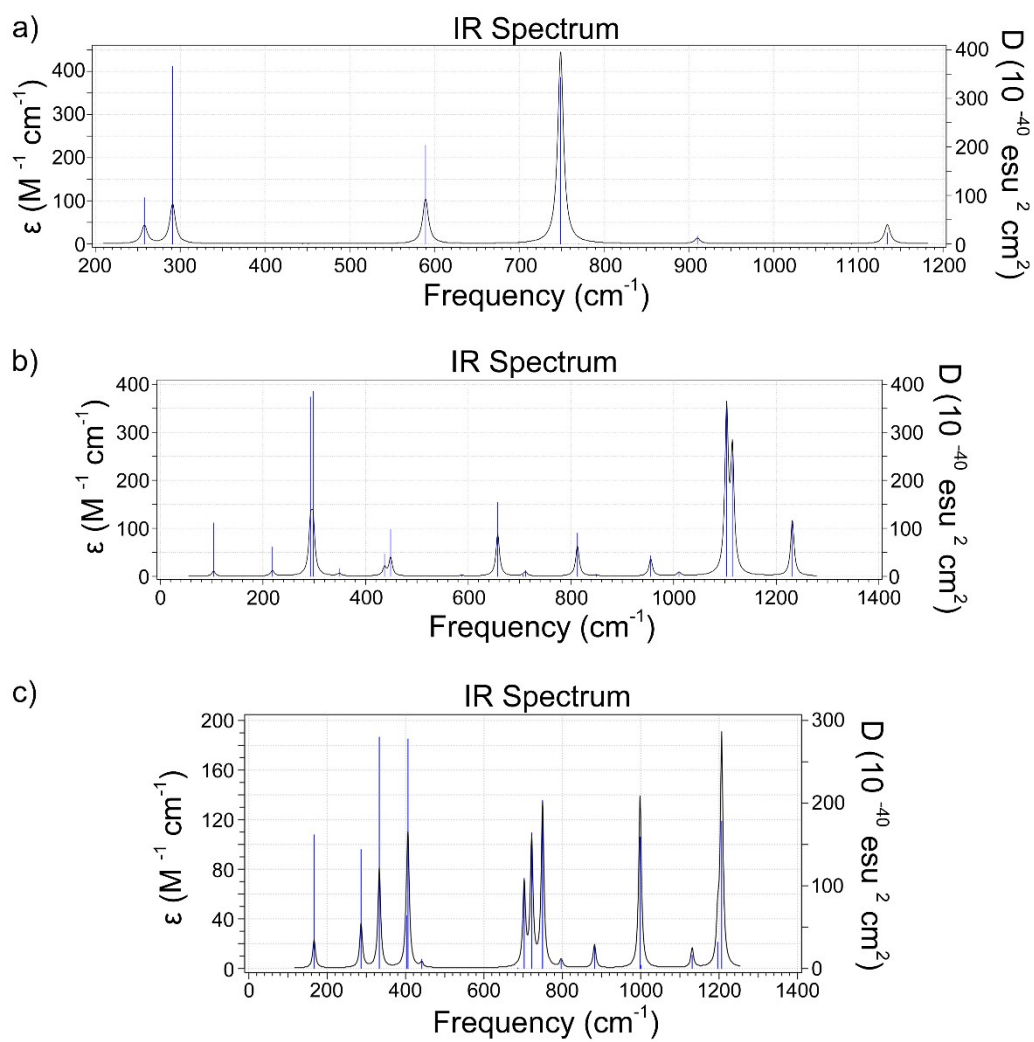


Figure S4. Infrared spectra of the a) global minimum structure, b) local minimum structure, and c) transition state structure of SnB_7^- .