Electronic Supplementary Material (ESI) for Nanoscale Advances.

Perfect Cubic Aromatic Metallo-Borospherenes TM_8B_6 (TM = Ni, Pd, Pt) As Superatoms Matching the 18-Electron Rule

Mei-Zhen Ao,[a,b] Yuan-Yuan Ma,[c] Yue-Wen Mu,*[a] and Si-Dian Li*[a]

[a]*Institute of Molecular Science, Shanxi University, Taiyuan 030006, China.*

[b]*Fenyang College of Shanxi Medical University, Fenyang 032200, China*

[c]*Shanxi Institute of Energy, Taiyuan 030006, China*

**E-mail: ywmu@sxu.edu.cn and lisidian@sxu.edu.cn*

Table of Contents

Figure S1. Low-lying isomers of Ni_8B_6 with its relative energies indicated in eV at PBE0 and TPSSh (parentheses) levels, respectively.

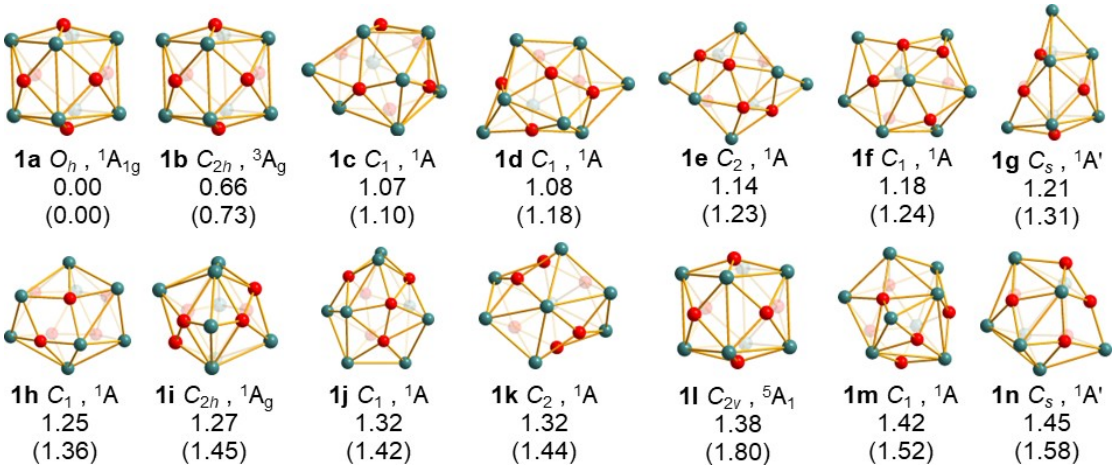

Figure S2. Low-lying isomers of Pd_8B_6 with its relative energies indicated in eV at PBE0 and TPSSh (parentheses) levels, respectively.

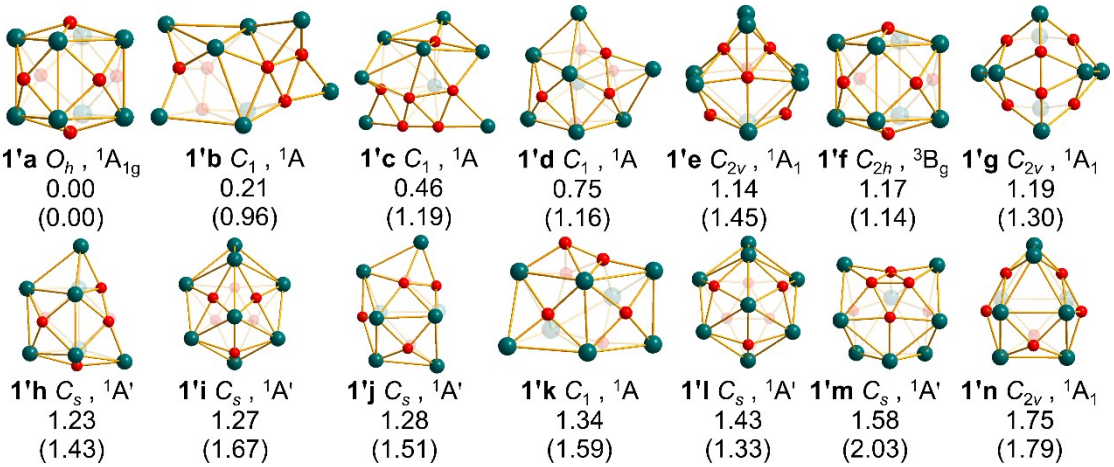

Figure S3. Low-lying isomers of Pt_8B_6 with its relative energies indicated in eV at PBE0 and TPSSh (parentheses) levels, respectively.

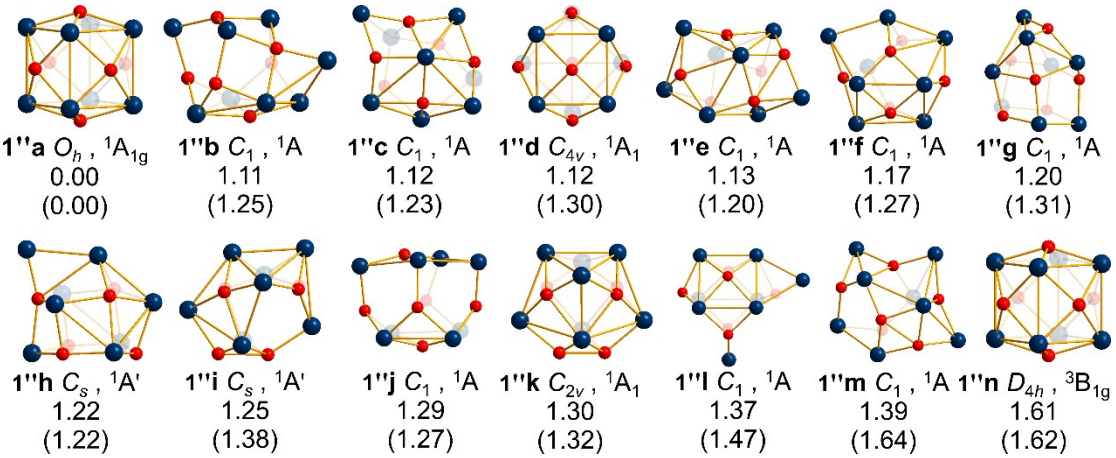

Figure S4. Low-lying isomers of monoanion $Ni_8B_6^{-1}$ with its relative energies indicated in eV at PBE0 and TPSSh (parentheses) levels, respectively.

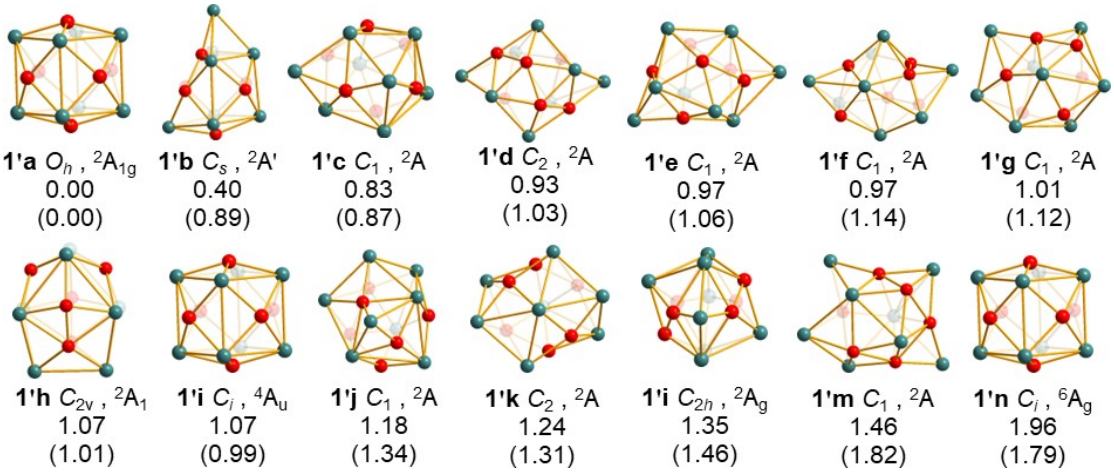

Figure S5. BOMD simulations of (a) O_h Ni_6B_6 (**1**), (b) O_h Pd_6B_6 (**2**), and (c) O_h Pt_6B_6 (**3**) at different temperatures with the RMSD and MAXD indicated in Å.

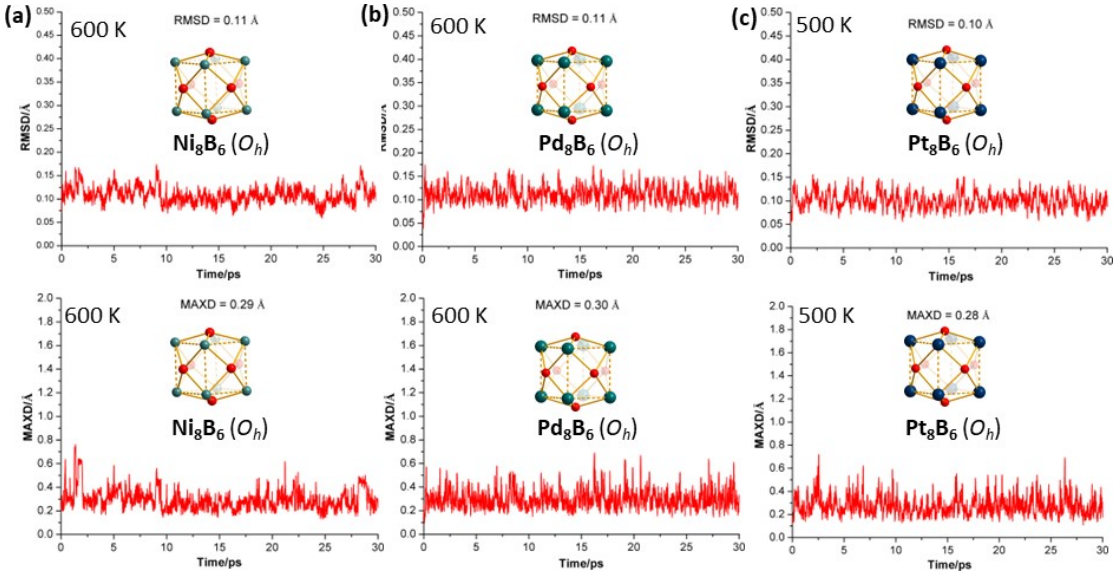

Figure S6 (a) The $1S^21P^61D^{10}$ 18-electron configurations of O_h Pd_8B_6 (**2**) and O_h Pt_8B_6 (**3**). The black and red solid lines refer to occupied and unoccupied orbitals, respectively. (b) AdNDP bonding patterns of O_h Pd_8B_6 (**2**) and O_h Pt_8B_6 (**3**) with the occupation numbers (ONs) indicated.

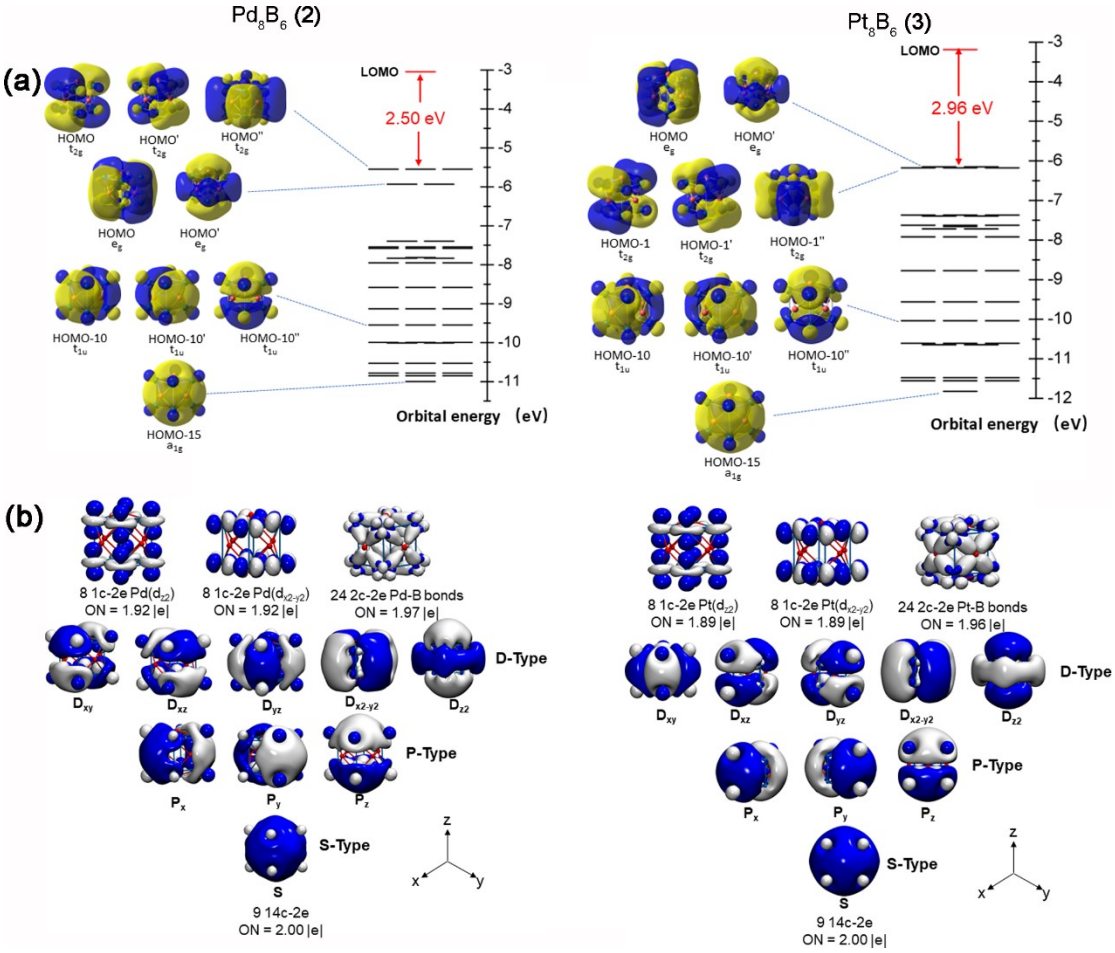

Figure S7. Simulated IR, Raman and UV-vis spectra of (a) O_h Pd_8B_6 and (b) O_h Pt_8B_6 at PBE0/6-311+G(d) level.

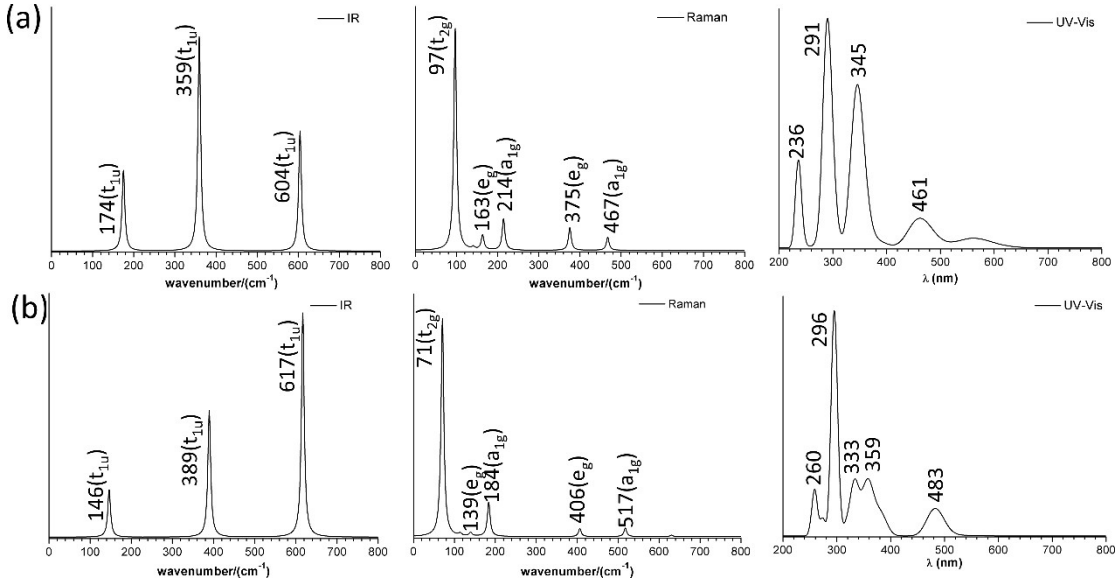

Table S1. Optimized cartesian coordinates (x, y, z) of (a) O_h Ni_6B_6 (**1**), (b) O_h Pd_6B_6 (**1'**), (c) O_h Pt_6B_6 (**1''**), and (d) O_h $Ni_8B_6^{-1}$ (**2**) at PBE0/6-311+G(d) level.

(a) O_h Ni_6 B_6 (**1**)

B	0.00000000	0.00000000	1.79487300
B	0.00000000	1.79487300	0.00000000
B	0.00000000	0.00000000	-1.79487300
B	0.00000000	-1.79487300	0.00000000
B	1.79487300	0.00000000	0.00000000
B	-1.79487300	0.00000000	0.00000000
Ni	-1.30575600	1.30575600	1.30575600
Ni	1.30575600	1.30575600	1.30575600
Ni	1.30575600	1.30575600	-1.30575600
Ni	-1.30575600	1.30575600	-1.30575600
Ni	-1.30575600	-1.30575600	-1.30575600
Ni	-1.30575600	-1.30575600	1.30575600
Ni	1.30575600	-1.30575600	-1.30575600
Ni	1.30575600	-1.30575600	1.30575600

(b) O_h Pd_6B_6 (**2**)

B	0.00000000	0.00000000	1.97396900
B	0.00000000	1.97396900	0.00000000
B	0.00000000	0.00000000	-1.97396900
B	0.00000000	-1.97396900	0.00000000
B	1.97396900	0.00000000	0.00000000
B	-1.97396900	0.00000000	0.00000000
Pd	-1.40539300	1.40539300	1.40539300
Pd	1.40539300	1.40539300	1.40539300
Pd	-1.40539300	-1.40539300	1.40539300
Pd	1.40539300	-1.40539300	-1.40539300
Pd	-1.40539300	-1.40539300	-1.40539300
Pd	-1.40539300	1.40539300	-1.40539300
Pd	1.40539300	1.40539300	-1.40539300
Pd	1.40539300	-1.40539300	1.40539300

(c) O_h Pt_6B_6 (**3**)

Pt	1.40832700	-1.40832700	-1.40832700
Pt	1.40832700	-1.40832700	1.40832700
Pt	1.40832700	1.40832700	1.40832700
Pt	1.40832700	1.40832700	-1.40832700
Pt	-1.40832700	-1.40832700	-1.40832700
Pt	-1.40832700	-1.40832700	1.40832700
Pt	-1.40832700	1.40832700	1.40832700
Pt	-1.40832700	1.40832700	-1.40832700
B	0.00000000	0.00000000	2.00454300
B	0.00000000	2.00454300	0.00000000
B	0.00000000	0.00000000	-2.00454300
B	0.00000000	-2.00454300	0.00000000
B	2.00454300	0.00000000	0.00000000
B	-2.00454300	0.00000000	0.00000000

(d) O_h $Ni_8B_6^{-1}$ (**1'**)

B	0.00000000	0.00000000	1.79487300
B	0.00000000	1.79487300	0.00000000

B	0.00000000	0.00000000	-1.79487300
B	0.00000000	-1.79487300	0.00000000
B	1.79487300	0.00000000	0.00000000
B	-1.79487300	0.00000000	0.00000000
Ni	-1.30575600	1.30575600	1.30575600
Ni	1.30575600	1.30575600	1.30575600
Ni	1.30575600	1.30575600	-1.30575600
Ni	-1.30575600	1.30575600	-1.30575600
Ni	-1.30575600	-1.30575600	-1.30575600
Ni	-1.30575600	-1.30575600	1.30575600
Ni	1.30575600	-1.30575600	-1.30575600
Ni	1.30575600	-1.30575600	1.30575600