SUPPLEMENTARY INFORMATION

BPt_4S_4 cluster: a planar tetracoordinate boron system with three charges all at their global energy minima

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Figure S1. Optimized structures of the GM **1-3** of $BPt_4S_4^n$ (n= -2, -1, 0) and three lowest-lying structures at the B3LYP/def2-TZVP level. Relative energies are listed in kcal mol^{-1} at the single-point CCSD(T)/def2-TZVP level, with ZPE corrections at B3LYP/def2-TZVP. The minimum frequencies are listed in cm^{-1}.

Figure S2. Detail Wiberg bond indices (WBIs) and Natural Population Analysis (NPA) charges (in $|e|$; red color) for **3** of BPt_4S_4 cluster from natural bond orbital (NBO) analyses.

Figure S3. Canonical molecular orbitals (CMOs) of $BPt_4S_4^-$ (**2**).

Figure S4. Chemical bonding analyses using AdNDP for the D_{4h} $BPt_4S_4^-$. ON stands for occupation number.

Table S1. Cartesian coordinates for optimized structures of clusters **1-3**, three low-lying isomers ***n*B-*n*D** (n = 1-3), at the B3LYP/def2-TZVP level.

Table S2. Cartesian coordinates for optimized structures of clusters BPt_4S_4H, BPt_4S_4Li and BPt_4S_4Na optimized at B3LYP/def2-TZVP level.

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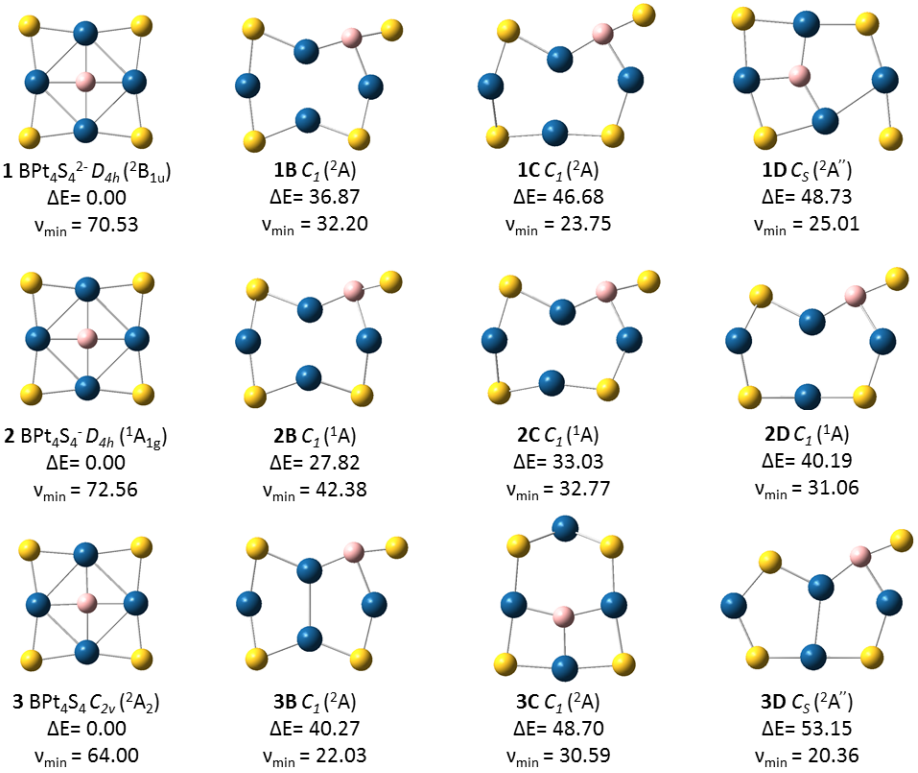

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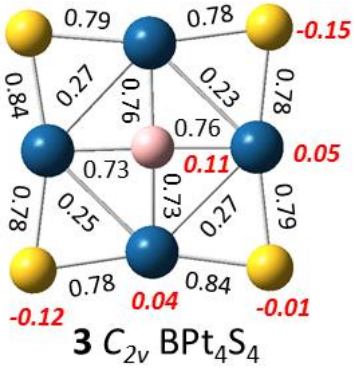

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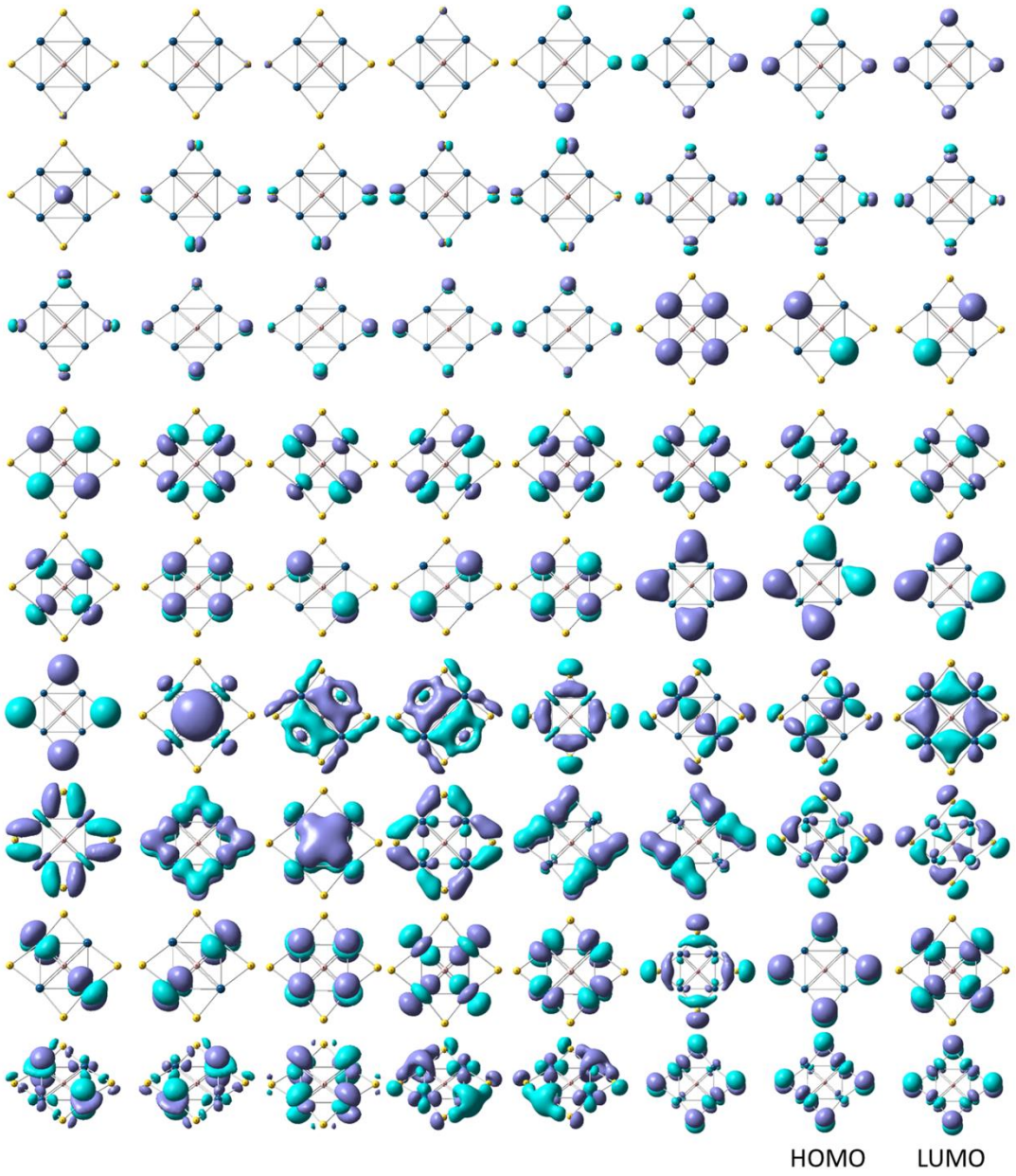

Figure S4. Chemical bonding analyses using AdNDP for the D_{4h} $BPt_4S_4^-$. ON stands for occupation number.

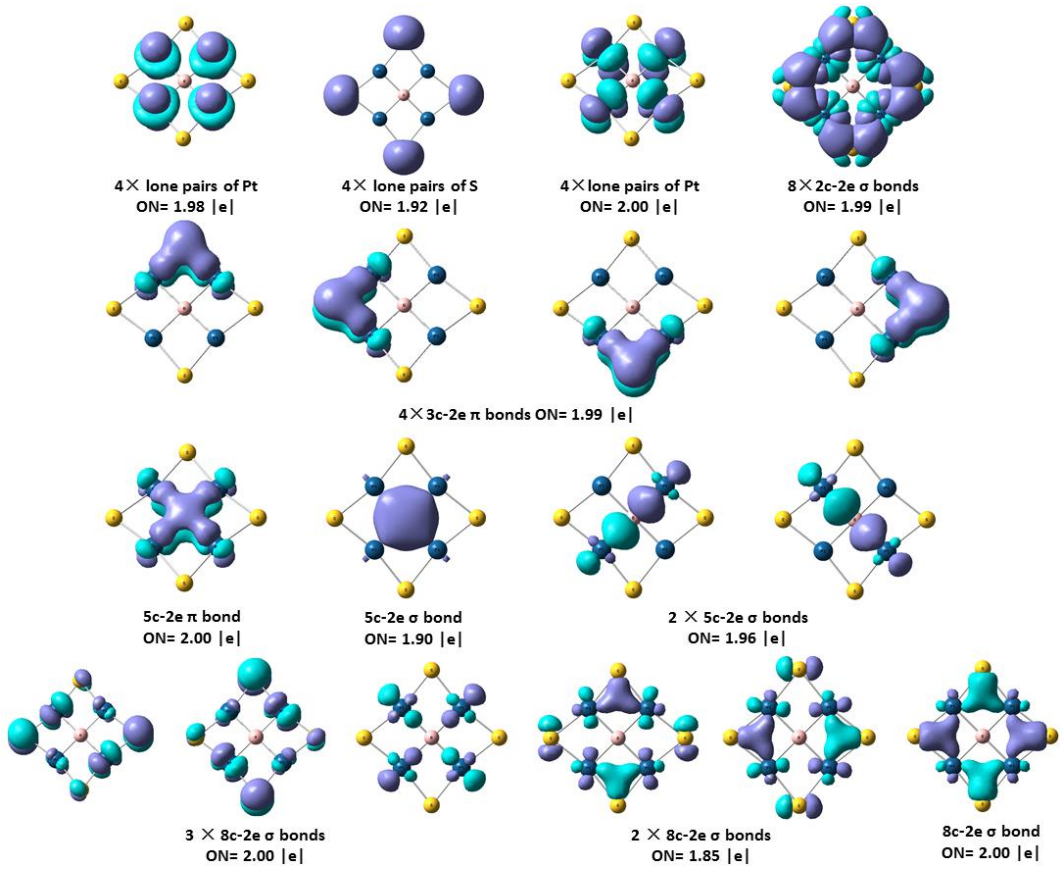

Table S1. Cartesian coordinates for optimized structures of clusters **1-3**, three low-lying isomers ***n*B-*n*D** (n = 1-3), at the B3LYP/def2-TZVP level.

1 (D_{4h}, $^2B_{1u}$)

B	0.00000000	0.00000000	0.00000000
Pt	0.00000000	1.99546700	0.00000000
Pt	1.99546700	0.00000000	0.00000000
Pt	−1.99546700	0.00000000	0.00000000
Pt	0.00000000	−1.99546700	0.00000000
S	2.29901600	2.29901600	0.00000000
S	−2.29901600	−2.29901600	0.00000000
S	−2.29901600	2.29901600	0.00000000
S	2.29901600	−2.29901600	0.00000000

1B (C_1, ^2A)

B	1.78706100	1.78244200	0.03844700
Pt	−0.06044200	1.34631100	0.23574800
Pt	−0.16903900	−1.39530500	0.02319100
Pt	2.42530600	−0.21797700	−0.10599500
Pt	−2.46997300	0.14959200	−0.15225500
S	−2.34240600	−2.09765400	−0.21288900
S	3.42768200	2.01125600	−0.48732400
S	1.80335200	−2.29003600	0.53759800
S	−2.11061100	2.39164200	0.14723600

1C (C_1, ^2A)

B	1.98517700	−1.66161000	0.18059800
Pt	0.18037000	−1.04884100	0.02550900
Pt	−2.62186100	−0.59388700	−0.21780600
Pt	2.69386200	0.24808300	−0.07048600
Pt	−0.57088500	1.68258900	0.08233200
S	3.67271600	−2.04940200	0.23072300
S	−2.78392800	1.44860500	0.59941400
S	1.59866700	2.18965100	−0.30215800
S	−1.55506900	−2.47332400	0.29527900

1D (C_S, $^2A''$)

B	0.00000000	−0.00074700	0.00000000
Pt	−1.50377100	−1.31221000	0.00000000
Pt	−1.31239900	1.50453600	0.00000000
Pt	1.31214000	−1.50258000	0.00000000
Pt	1.50364500	1.31065300	0.00000000
S	−3.24297100	0.21989800	0.00000000
S	0.22052900	3.24417100	0.00000000
S	−0.22079500	−3.24470700	0.00000000
S	3.24511500	−0.22107400	0.00000000

2 (D_{4h}, $^1A_{1g}$)

B	0.00000000	0.00000000	−0.00000000

Pt	0.00000000	2.00344000	0.00000000
Pt	0.00000000	−2.00344000	0.00000000
Pt	2.00344000	0.00000000	0.00000000
Pt	−2.00344000	0.00000000	0.00000000
S	2.26768600	2.26768600	0.00000000
S	−2.26768600	2.26768600	0.00000000
S	−2.26768600	−2.26768600	0.00000000
S	2.26768600	−2.26768600	0.00000000

2B (C_1, ^{1}A)

B	1.85533800	−1.82920400	0.08634500
Pt	2.32309800	0.23104800	−0.14280500
Pt	0.02446800	−1.31205200	0.28595200
Pt	−0.19653900	1.43206600	0.00478900
Pt	−2.44140500	−0.22137600	−0.24237400
S	1.75700200	2.22911900	0.68480700
S	−1.99756000	−2.34237300	0.34213300
S	−2.36677700	1.96890700	−0.03043800
S	3.44313700	−1.91624700	−0.56309800

2C (C_1, ^{1}A)

B	2.06600400	−1.65225400	0.16412500
Pt	0.24810100	−1.13256300	−0.10663700
Pt	2.59834200	0.36111100	0.03531800
Pt	−2.53327500	−0.50004200	−0.10066100
Pt	−0.64727300	1.51241800	−0.04699500
S	−1.54329700	−2.48466800	0.08225200
S	3.75806300	−1.78462100	0.39411100
S	1.42058600	2.18743200	−0.42677000
S	−2.65221400	1.42367900	0.96661800

2D (C_1, ^{1}A)

B	1.87264400	−1.75820100	0.24616400
Pt	−0.40326600	1.79864200	0.24104500
Pt	−2.72537500	−0.62201000	−0.35105700
Pt	2.67706200	0.09692300	−0.22181000
Pt	0.12527100	−0.99761400	0.20170400
S	−2.57955200	1.54108000	0.04389800
S	−1.66379300	−2.23555700	0.69835600
S	1.72973500	2.09154300	−0.20279900
S	3.51916300	−2.19283800	0.01794200

3 (C_{2v}, ^{2}A$_2$)

B	0.00000000	0.00000000	−0.03077000
Pt	0.00000000	1.38472700	1.40321200
Pt	0.00000000	1.42005100	−1.41426100
Pt	0.00000000	−1.38472700	1.40321200
Pt	0.00000000	−1.42005100	−1.41426100

S	0.00000000	0.00000000	3.22358000
S	0.00000000	3.19369000	0.05250100
S	0.00000000	-3.19369000	0.05250100
S	0.00000000	0.00000000	-3.21123300

3B (C_1, ^{2}A)

B	-1.80449000	-1.88755200	0.13051900
Pt	0.00543900	-1.30453000	0.01362300
Pt	-2.42574100	0.23989100	-0.04963000
Pt	2.49797200	-0.19845600	-0.08990400
Pt	0.22197800	1.37522100	0.00509700
S	1.97529000	-2.35466100	0.19395500
S	-3.49889200	-1.93387400	0.04573400
S	2.36035000	1.98583300	0.21674400
S	-1.73362500	2.34594300	0.09174800

3C (C_1, ^{2}A)

B	0.57124600	-0.02759300	0.14757900
Pt	0.07840200	-1.92300800	0.21300200
Pt	0.16642100	1.90489500	0.26088400
Pt	2.50998300	-0.02475500	-0.23232200
Pt	-2.90306200	0.02251000	-0.40537700
S	2.31635100	-2.29001300	-0.18345100
S	-2.05978900	1.85269500	0.41626300
S	2.40290400	2.23317300	-0.18419300
S	-2.11523000	-1.68798700	0.70385000

3D (C_S, ^{2}A$''$)

B	-1.28562000	2.35375500	0.00000000
Pt	3.18331500	-0.36442000	0.00000000
Pt	-2.68995900	0.80821600	0.00000000
Pt	-0.18322100	-1.76744800	0.00000000
Pt	0.00000000	0.92185500	0.00000000
S	-2.73512800	3.24185700	0.00000000
S	2.09852300	1.53329200	0.00000000
S	-2.41028500	-1.38518300	0.00000000
S	1.93674100	-2.16675200	0.00000000

Table S2. Cartesian coordinates for optimized structures of clusters BPt_4S_4H, BPt_4S_4Li and BPt_4S_4Na optimized at B3LYP/def2-TZVP level.

BPt_4S_4H (C_S)

B	0.02520300	0.00032000	0.08011600
Pt	0.01231200	-1.95753800	-0.04169000
Pt	0.02207400	1.95807100	-0.04186000
Pt	2.03355900	-0.00492600	0.03557500
Pt	-2.05893400	0.00423700	0.07335400
S	2.31457000	-2.25649700	0.00581700
S	-2.27833800	-2.30848700	-0.12975200
S	-2.26693500	2.31926200	-0.13074700
S	2.32576400	2.24520400	0.00714300
H	-2.34985000	0.01874900	1.58043300

BPt_4S_4Li (C_{4v})

B	0.00014100	0.00018300	-0.39493100
Pt	1.97418000	0.02624200	-0.02416700
Pt	-1.97473900	-0.02635000	-0.02440300
Pt	-0.02602300	1.97444100	-0.02449800
Pt	0.02657400	-1.97429400	-0.02464600
S	2.25870100	2.31958100	0.06227100
S	2.31935100	-2.25896500	0.06250700
S	-2.25866900	-2.31881600	0.06295600
S	-2.31930600	2.25814000	0.06273700
Li	-0.00044400	-0.00100800	1.86290900

BPt_4S_4Na (C_{4V})

B	0.00092300	0.00001600	-0.38000800
Pt	1.98233600	-0.08569800	-0.07448800
Pt	-1.97959900	0.08562100	-0.07713400
Pt	0.08540400	1.98091600	-0.07574800
Pt	-0.08591900	-1.98092400	-0.07575900
S	2.38717500	2.18873400	0.01851000
S	2.18923400	-2.38660400	0.01854100
S	-2.38738900	-2.19005500	0.01882400
S	-2.18962800	2.38787700	0.01881400
Na	-0.01529000	0.00066200	2.21354500