

Electronic Supplementary Information

**M@B<sub>7</sub>O<sub>7</sub><sup>±</sup> (M = Ni, Pd, Pt): Aromatic molecular stars with a planar heptacoordinate transition metal**

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Contents

**SI1:** The results for the electronic structure analysis, the distribution of NICS values, the potential energy surface explorations, and the BOMD simulations of M@B<sub>7</sub>O<sub>7</sub><sup>-/+</sup> (M = Ni, Pd, Pt).

**Fig. S1–S2.** AdNDP bonding patterns of Ni@B<sub>7</sub>O<sub>7</sub><sup>+(1)</sup>, Ni@B<sub>7</sub>O<sub>7</sub><sup>-(1')</sup>, Pd@B<sub>7</sub>O<sub>7</sub><sup>+(2)</sup> and Pd@B<sub>7</sub>O<sub>7</sub><sup>-(2')</sup>. Only one orbital is showed when multiple orbitals in a pattern are identical due to molecular symmetry.

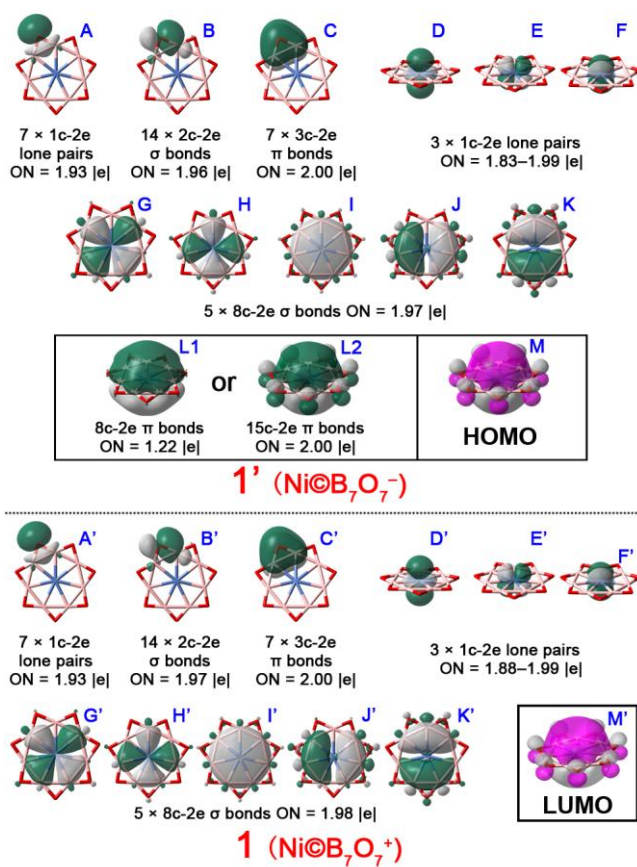
**Fig. S3–S4.** The distribution of NICS values for 1', 1, 2', and 2. Panels A and C correspond to the molecular planes, while panels B and D correspond to the planes parallel to and located 1 Å above the molecular planes. The NICS values that are negative, positive, and close to zero indicate aromaticity, anti-aromaticity, and non-aromaticity, respectively.

**Fig. S5.** Structures and relative energies (ΔE, in kcal mol<sup>-1</sup> at the CCSD(T)//PBE0 level) of M@B<sub>7</sub>O<sub>7</sub><sup>-/+</sup> (M = Ni, Pd, Pt) and their low-energy isomers.

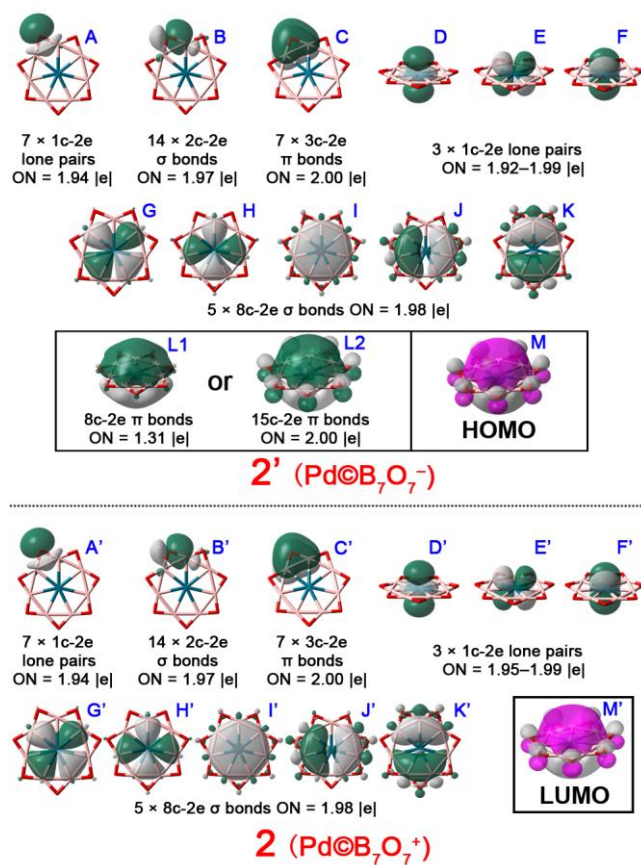
**Fig. S6–S7.** RMSD (in Å) versus simulation time (in ps) for the BOMD simulation of M@B<sub>7</sub>O<sub>7</sub><sup>±</sup> (M = Ni, Pd, Pt) at the PBE/DZVP level. The examined temperatures include 298, and 1000 K.

**SI2:** Cartesian coordinates of PBE0/BS1-optimized structures shown in Fig. S5

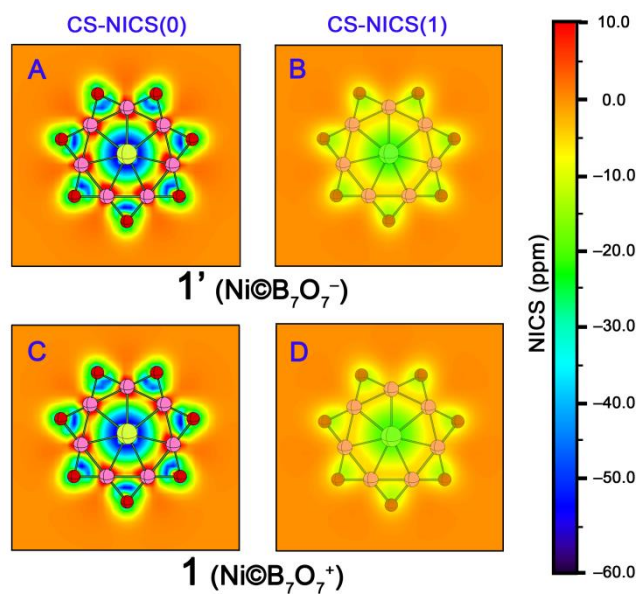
**SI1:** The results for the electronic structure analysis, the distribution of NICS values, the potential energy surface explorations, and the BOMD simulations of  $M@B_7O_7^{-/+}$  ( $M = Ni, Pd, Pt$ ).



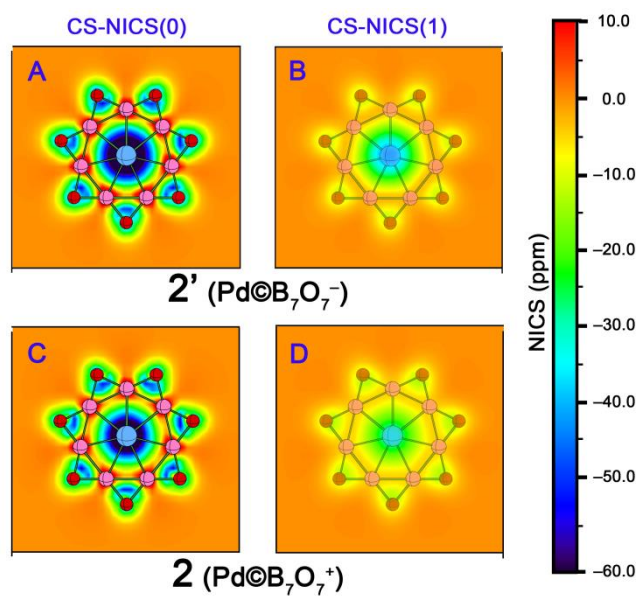
**Fig. S1.** AdNDP bonding patterns of  $Ni@B_7O_7^-$  (**1'**) and  $Ni@B_7O_7^+$  (**1**). Only one orbital is shown when multiple orbitals in a pattern are identical due to molecular symmetry.



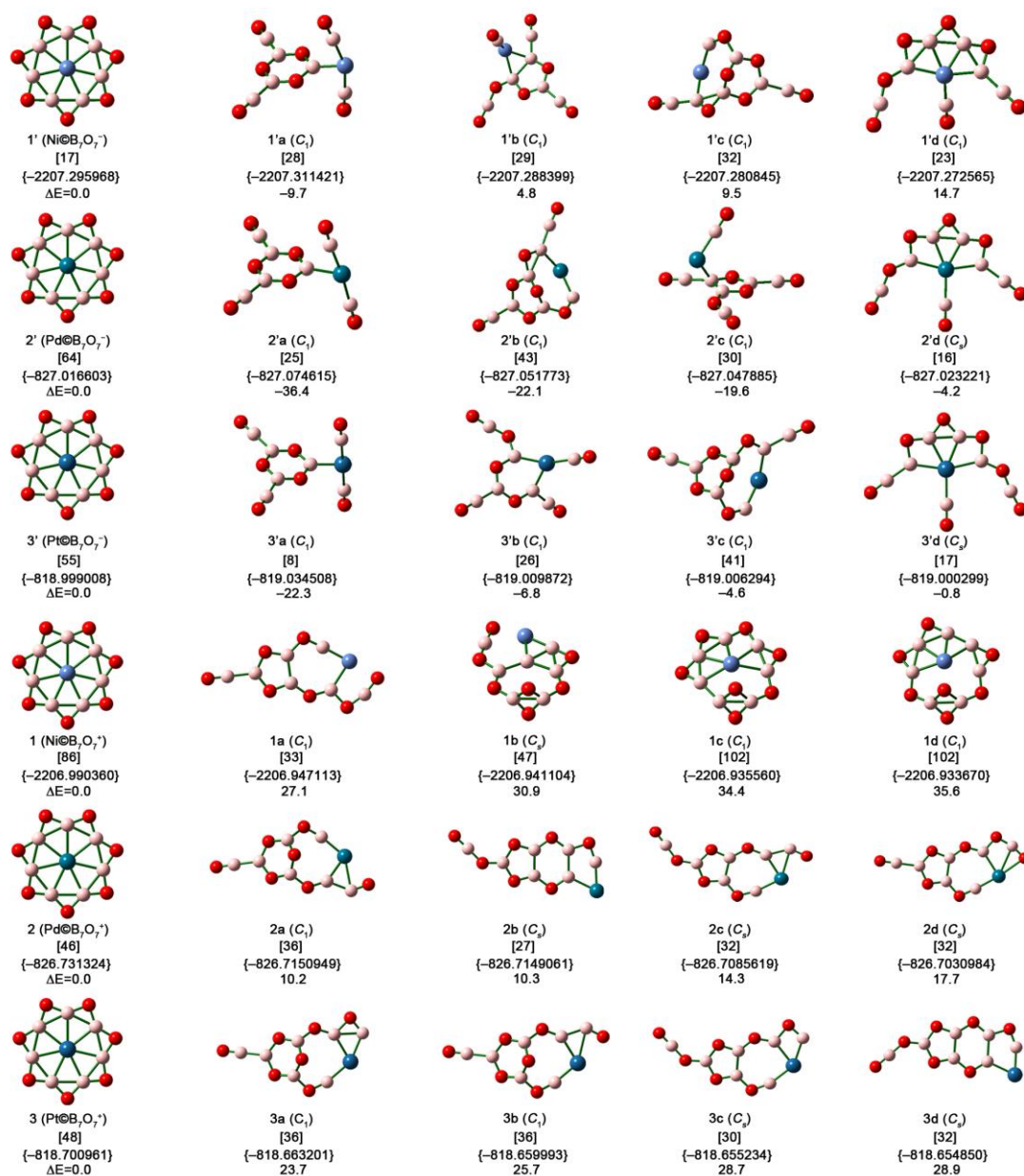
**Fig. S2.** AdNDP bonding patterns of Pd@B<sub>7</sub>O<sub>7</sub><sup>-</sup>(**2'**) and Pd@B<sub>7</sub>O<sub>7</sub><sup>+</sup>(**2**). Only one orbital is showed when multiple orbitals in a pattern are identical due to molecular symmetry.



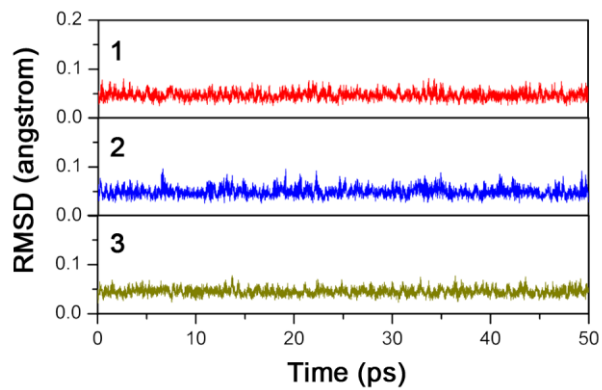
**Fig. S3.** The distribution of NICS values for  $1'$  and  $1$ . Panels A and C correspond to the molecular planes, while panels B and D correspond to the planes parallel to and located 1 Å above the molecular planes. The NICS values that are negative, positive, and close to zero indicate aromaticity, anti-aromaticity, and non-aromaticity, respectively.



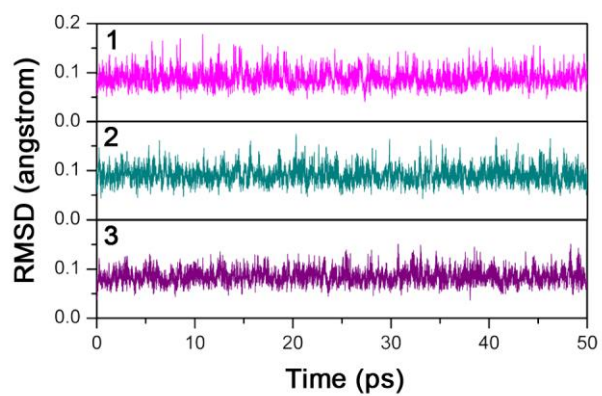
**Fig. S4.** The distribution of NICS values for  $2'$  and  $2$ . Panels A and C correspond to the molecular planes, while panels B and D correspond to the planes parallel to and located 1 Å above the molecular planes. The NICS values that are negative, positive, and close to zero indicate aromaticity, anti-aromaticity, and non-aromaticity, respectively.



**Fig. S5.** Structures and relative energies ( $\Delta E$ , in kcal mol<sup>-1</sup> at the CCSD(T)//PBE0 level) of M@B<sub>7</sub>O<sub>7</sub><sup>-/+</sup> (M = Ni, Pd, Pt) and their low-energy isomers. The lowest harmonic frequencies (in cm<sup>-1</sup> at the PBE0 level) of all clusters are given in square brackets, and whose total energies expressed as a value in curly brackets (in a.u. at the CCSD(T)//PBE0 level).



**Fig. S6.** RMSD (in Å) versus simulation time (in ps) for the BOMD simulation of  $M@B_7O_7^+$  ( $M = Ni, Pd, Pt$ ) at the PBE/DZVP level and 298 K.



**Fig. S7.** RMSD (in Å) versus simulation time (in ps) for the BOMD simulation of  $M@B_7O_7^+$  ( $M = Ni, Pd, Pt$ ) at the PBE/DZVP level and 1000 K.

**SI2:** Cartesian coordinates of PBE0/BS1-optimized structures shown in Fig. S5Ni@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (**1'**)

B	0.00000000	2.01687400	0.00000000
B	-1.57685600	1.25750000	0.00000000
B	-1.96630700	-0.44879700	0.00000000
B	1.57685600	1.25750000	0.00000000
B	1.96630700	-0.44879700	0.00000000
B	0.87508900	-1.81714100	0.00000000
B	-0.87508900	-1.81714100	0.00000000
O	-2.26509200	-1.80635100	0.00000000
O	-1.25703100	2.61025300	0.00000000
O	-2.82452400	0.64467900	0.00000000
O	1.25703100	2.61025300	0.00000000
O	2.26509200	-1.80635100	0.00000000
O	0.00000000	-2.89716200	0.00000000
O	2.82452400	0.64467900	0.00000000
Ni	0.00000000	0.00000000	0.00000000

Pd@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (**2'**)

B	0.00000000	2.09309900	0.00000000
B	-1.63645100	1.30502600	0.00000000
B	-2.04062100	-0.46575800	0.00000000
B	1.63645100	1.30502600	0.00000000
B	2.04062100	-0.46575800	0.00000000
B	0.90816200	-1.88581700	0.00000000
B	-0.90816200	-1.88581700	0.00000000
O	-2.30691200	-1.83970100	0.00000000
O	-1.28024000	2.65844500	0.00000000
O	-2.87667300	0.65658200	0.00000000
O	1.28024000	2.65844500	0.00000000
O	2.30691200	-1.83970100	0.00000000
O	0.00000000	-2.95065200	0.00000000
O	2.87667300	0.65658200	0.00000000
Pd	0.00000000	0.00000000	0.00000000

Pt@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (**3'**)

B	0.00000000	2.12503800	0.00000000
B	1.66142100	1.32493900	0.00000000
B	2.07175800	-0.47286500	0.00000000
B	-1.66142100	1.32493900	0.00000000
B	-2.07175800	-0.47286500	0.00000000
B	-0.92201900	-1.91459300	0.00000000
B	0.92201900	-1.91459300	0.00000000
O	2.32746900	-1.85609400	0.00000000

O	1.29164800	2.68213400	0.00000000
O	2.90230600	0.66243200	0.00000000
O	-1.29164800	2.68213400	0.00000000
O	-2.32746900	-1.85609400	0.00000000
O	0.00000000	-2.97694400	0.00000000
O	-2.90230600	0.66243200	0.00000000
Pt	0.00000000	0.00000000	0.00000000

Ni@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (1)

B	0.00000000	2.08990500	0.00000000
B	1.63395300	1.30303400	0.00000000
B	2.03750600	-0.46504800	0.00000000
B	-1.63395300	1.30303400	0.00000000
B	-2.03750600	-0.46504800	0.00000000
B	-0.90677600	-1.88293900	0.00000000
B	0.90677600	-1.88293900	0.00000000
O	2.26786900	-1.80856500	0.00000000
O	1.25857200	2.61345200	0.00000000
O	2.82798600	0.64546900	0.00000000
O	-1.25857200	2.61345200	0.00000000
O	-2.26786900	-1.80856500	0.00000000
O	0.00000000	-2.90071300	0.00000000
O	-2.82798600	0.64546900	0.00000000
Ni	0.00000000	0.00000000	0.00000000

Pd@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (2)

B	0.00000000	2.15903000	0.00000000
B	1.68799800	1.34613300	0.00000000
B	2.10489900	-0.48042900	0.00000000
B	-1.68799800	1.34613300	0.00000000
B	-2.10489900	-0.48042900	0.00000000
B	-0.93676800	-1.94521900	0.00000000
B	0.93676800	-1.94521900	0.00000000
O	2.30375200	-1.83718100	0.00000000
O	1.27848600	2.65480300	0.00000000
O	2.87273100	0.65568200	0.00000000
O	-1.27848600	2.65480300	0.00000000
O	-2.30375200	-1.83718100	0.00000000
O	0.00000000	-2.94660900	0.00000000
O	-2.87273100	0.65568200	0.00000000
Pd	0.00000000	0.00000000	0.00000000

Pt@B<sub>7</sub>O<sub>7</sub><sup>-</sup> (3)

B	0.00000000	2.16915700	0.00000000
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B	1.69591500	1.35244700	0.00000000
B	2.11477200	-0.48268300	0.00000000
B	-1.69591500	1.35244700	0.00000000
B	-2.11477200	-0.48268300	0.00000000
B	-0.94116200	-1.95434300	0.00000000
B	0.94116200	-1.95434300	0.00000000
O	2.30858700	-1.84103700	0.00000000
O	1.28116900	2.66037500	0.00000000
O	2.87876100	0.65705800	0.00000000
O	-1.28116900	2.66037500	0.00000000
O	-2.30858700	-1.84103700	0.00000000
O	0.00000000	-2.95279400	0.00000000
O	-2.87876100	0.65705800	0.00000000
Pt	0.00000000	0.00000000	0.00000000

**(1'a)**

B	1.61763500	1.17834000	-0.00017500
B	-0.49262200	0.00000400	0.00032100
B	2.48240100	2.63802100	-0.00030700
B	-1.95769000	-0.00000800	1.90850100
B	1.61762900	-1.17834500	-0.00019700
B	2.48238600	-2.63803100	-0.00039200
B	-1.95903600	0.00003400	-1.90824500
O	3.10960700	3.66675400	-0.00036400
O	0.27500800	1.19025800	0.00021600
O	-1.70359600	0.00009700	-3.10159800
O	2.33575100	-0.00000400	-0.00036000
O	3.10959000	-3.66676500	-0.00048100
O	-1.70162800	-0.00008400	3.10171400
O	0.27500200	-1.19025500	0.00019300
Ni	-2.30540600	-0.00000300	0.00028300

**(1'b)**

B	1.77420300	-1.14193300	0.06400800
B	-0.37561700	-0.88737000	0.78035500
B	3.18352600	-1.98374900	-0.33724200
B	-2.06822200	-0.11018300	-1.85977100
B	0.41821700	0.68962700	0.28864900
B	1.30480000	3.01819500	0.33845400
B	-1.82061300	-1.25768200	1.54001900
O	4.19209300	-2.58673000	-0.60553100
O	0.70383200	-1.78579700	0.60317700
O	-2.87671700	-1.42163100	2.12385600
O	1.68234600	0.20943500	-0.11119000

O	2.07356600	3.95282100	0.20986400
O	-2.37950700	-0.35479600	-3.01220200
O	0.40688100	2.08378500	0.52870300
Ni	-1.51790800	0.27102800	-0.07020600

**(1'c)**

B	-3.11914900	-1.21456100	-0.06829700
B	0.04813900	-0.52603600	0.94248700
B	-0.68553000	2.09792800	-0.54277500
B	2.22549000	-0.35866900	-0.03436300
B	-1.60476600	-0.97967400	0.56072100
B	0.95010100	1.44101200	0.64114500
B	3.67247800	-1.02316700	-0.62379400
O	2.10570500	1.02089200	0.00027800
O	0.31428900	2.61890300	0.16058500
O	-4.15759300	-1.28517600	-0.69946600
O	-0.87645400	-1.39643300	1.62252000
O	1.22853200	-1.16203100	0.35092700
O	4.70589300	-1.49623900	-1.03140200
O	0.42237500	0.69656300	1.64123800
Ni	-1.33485000	0.38728600	-0.74046700

**(1'd)**

B	2.13398800	0.09514700	-0.04144600
B	0.01035600	1.57646100	1.02146800
B	1.44942400	-1.52147700	0.03739100
B	-0.30826900	-1.93205900	-0.06329000
B	-1.70101700	-0.76930700	-0.00889200
B	-3.43895600	0.91703900	-0.48406600
B	3.11346000	1.32812200	-0.62519700
O	-0.06452300	2.52806900	1.78169000
O	2.71538900	-1.14603000	0.37655400
O	3.78222100	2.21463600	-1.10262000
O	0.80802100	-2.75878000	0.01808400
O	-3.97444700	1.96528400	-0.78583100
O	-2.99388600	-0.28248500	-0.19496500
O	-1.63655300	-2.17320500	0.16155600
Ni	0.16483200	-0.04462600	-0.04341300

**(2'a)**

B	2.04252100	1.17905500	-0.18554500
B	-0.03273400	-0.00002500	0.17996700
B	2.89344400	2.63788200	-0.33480200
B	-1.12451500	-0.00011100	2.07861900

B	2.04256700	-1.17900900	-0.18557800
B	2.89360500	-2.63775600	-0.33496100
B	-2.62634800	0.00005800	-1.79294400
O	3.51385300	3.66450800	-0.44260500
O	0.71920300	1.18829200	0.05535200
O	-2.99354400	0.00012300	-2.95489300
O	2.74589000	0.00004200	-0.31772100
O	3.51412900	-3.66430300	-0.44285900
O	-0.75491600	-0.00014500	3.23849700
O	0.71925700	-1.18830400	0.05533300
Pd	-1.95986300	-0.00004700	0.20320400

**(2'b)**

B	-3.16105700	-1.53139300	0.12729700
B	0.17583400	-0.66678200	0.90427900
B	-0.24050400	2.30991500	-0.22991400
B	2.39432800	-0.53813500	0.00219100
B	-1.58839700	-1.06004300	0.47213500
B	1.26734800	1.25303100	0.92016100
B	3.79047600	-1.24192700	-0.65920300
O	2.41202700	0.81840400	0.27357000
O	0.77562800	2.54028900	0.59553500
O	-4.28843300	-1.78572900	-0.24104200
O	-0.78844000	-1.56643800	1.44454500
O	1.30743000	-1.28695200	0.22409300
O	4.78863200	-1.74386700	-1.11612100
O	0.60653000	0.42112600	1.75952400
Pd	-1.12385100	0.61308700	-0.67838100

**(2'c)**

B	1.99573500	-0.87833400	0.42243200
B	-0.15998500	-0.54220300	1.07813700
B	3.45040100	-1.70231000	0.17148000
B	-1.12598600	-1.22357500	-1.82876300
B	0.58171100	0.86842700	0.43561700
B	1.06232900	3.25358600	-0.06780600
B	-1.53370500	-0.83864700	1.97979100
O	4.49838600	-2.27979300	0.02287700
O	0.93500600	-1.47996500	1.01311400
O	-2.56425600	-0.94057700	2.61767900
O	1.86826900	0.44754700	0.06684800
O	1.65402600	4.25085000	-0.43528700
O	-0.89473200	-2.01740100	-2.72361900
O	0.33990900	2.25185100	0.36974000

Pd	-1.47924700	0.07511300	-0.40011400
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**(2'd)**

B	2.32525600	0.01383600	-0.00046200
B	-0.14759800	2.08316500	-0.00027400
B	1.42093900	-1.65295600	-0.00009600
B	-0.32001300	-2.00565400	-0.00036200
B	-1.81744800	-0.80180500	-0.00034100
B	-3.79151100	0.72558700	0.00024400
B	3.53297000	1.19266100	0.00009200
O	-0.31753100	3.28974600	-0.00081000
O	2.74821700	-1.34250700	0.00070400
O	4.37907300	2.05535000	0.00042500
O	0.76275800	-2.87791300	0.00028600
O	-4.51777900	1.69913800	0.00081300
O	-3.15174200	-0.41848600	-0.00026200
O	-1.66518600	-2.21296900	-0.00043000
Pd	0.17575100	0.01493400	0.00000400

**(3'a)**

B	-2.43320600	-1.17914400	-0.13439100
B	-0.33413100	-0.00006700	0.01140300
B	-3.29457100	-2.63785000	-0.19981600
B	1.12225700	0.00028900	2.09830700
B	-2.43312200	1.17914900	-0.13472800
B	-3.29449000	2.63784500	-0.20030200
B	2.03663400	-0.00030400	-1.93692500
O	-3.92357000	-3.66351100	-0.25064100
O	-1.09050000	-1.18760400	-0.04933800
O	2.27940200	-0.00048600	-3.13128900
O	-3.14709600	0.00000600	-0.17590500
O	-3.92349800	3.66349600	-0.25121500
O	0.85015200	0.00043800	3.28679400
O	-1.09042700	1.18754700	-0.04982600
Pt	1.58355700	0.00001700	0.09555900

**(3'b)**

B	-2.00778900	-1.31394600	0.31537300
B	0.14809400	-1.26592300	-0.65405200
B	-3.30234100	-2.18047100	0.98373100
B	2.66135300	0.32550000	1.37561300
B	-0.96111600	0.77428200	-0.19213700
B	-2.46790100	2.69975000	-0.64300000
B	1.10716300	-1.83333200	-1.91531800

O	-4.22087300	-2.80241000	1.45434400
O	-0.94289600	-1.99784000	-0.18111600
O	1.80611800	-2.17259100	-2.84276500
O	-2.07667500	0.04184200	0.24360500
O	-3.48884700	3.35686500	-0.72249100
O	3.57889700	0.32657200	2.17477300
O	-1.31731600	2.07390900	-0.60336400
Pt	0.99237700	0.29948600	0.09570600

**(3'c)**

B	3.02866500	1.82672600	0.27420400
B	-0.40941100	0.77679300	0.90267700
B	-0.06082300	-2.15658700	-0.00630800
B	-2.64047400	0.62319200	0.01840300
B	1.47437600	1.19515200	0.46536000
B	-1.57303400	-1.09235900	1.11237600
B	-4.00801600	1.30855000	-0.71785300
O	-2.72610800	-0.68291600	0.46469800
O	-1.07841400	-2.38240100	0.83067500
O	4.15249000	2.20645400	0.02479800
O	0.56509300	1.70859600	1.34459700
O	-1.51347600	1.33812700	0.13755600
O	-4.98718400	1.79653700	-1.22712000
O	-0.86987400	-0.20468900	1.85764900
Pt	0.93081300	-0.54673100	-0.48342500

**(3'd)**

B	-2.28550000	-0.03975200	0.00021800
B	0.19573600	-2.06681000	0.00012100
B	-1.38946700	1.66598200	0.00040800
B	0.34469500	2.02262400	-0.00002900
B	1.84613300	0.79209500	-0.00047800
B	3.83634100	-0.72117500	0.00006400
B	-3.50730900	-1.20712000	-0.00017200
O	0.38055600	-3.27117400	0.00024900
O	-2.70917100	1.32199300	0.00053300
O	-4.36159900	-2.06175700	-0.00052800
O	-0.73869500	2.89592700	0.00051000
O	4.57027100	-1.68918600	0.00069500
O	3.18237700	0.41386500	-0.00072200
O	1.69361000	2.20729700	-0.00048800
Pt	-0.14541000	-0.00980700	-0.00003400

**(1a)**

B	-1.31706200	-1.01719000	0.00515400
B	3.26025600	-0.09416900	-0.00080200
B	1.35114200	1.02646000	0.00529800
B	-0.77817500	1.55323900	0.00490600
B	4.92123000	-0.31892600	-0.00377400
B	1.09355200	-0.65153200	0.00163200
B	-3.34555600	-1.23993100	0.00019200
O	-2.29713100	-2.03851800	0.01142800
O	0.40115500	2.06869300	0.00912500
O	-0.04115200	-1.41353700	0.00106000
O	-4.09414600	-0.25358800	-0.01050100
O	2.68708200	1.19453300	0.00189200
O	2.36013700	-1.15837600	-0.00222300
O	6.10757800	-0.47945800	-0.00589700
Ni	-2.38982600	0.72686600	-0.00364700

**(1b)**

B	2.32868600	-1.35004600	-0.00035000
B	2.84628400	0.29780600	0.00019900
B	-0.17434200	0.23985800	-0.00001600
B	-0.73143300	1.92070100	-0.00025400
B	0.05831000	-1.51528700	-0.00008400
B	-2.21570200	-1.66392200	0.00037600
B	1.05370400	1.63328400	0.00031400
O	1.23133600	-2.16589700	-0.00043700
O	2.78653200	-0.58675700	-1.07584000
O	2.78704700	-0.58756900	1.07553100
O	2.38928400	1.59394300	0.00062500
O	0.27443600	2.79332200	0.00010000
O	-1.09574400	-2.32673400	0.00017900
O	-3.18284800	-0.89089400	0.00060200
Ni	-2.04813800	0.69831200	-0.00025000

**(1c)**

B	-0.46322800	1.97596900	-0.04516500
B	-0.40842800	-2.02260700	-0.08108900
B	1.25827500	-1.83186900	-0.03438300
B	-1.90220000	0.73095100	-0.05701000
B	2.28491700	-0.35258300	-0.07127300
B	1.18665900	1.54130800	-0.04628400
B	-1.85532300	-1.13311100	-0.07947800
O	1.57628900	-0.92360800	1.03690200
O	-1.82589200	2.09000000	-0.14611000

O	-1.65475800	-2.46642100	-0.37051200
O	0.62244400	2.76120800	-0.30600600
O	-2.87058000	-0.22430000	-0.20209000
O	2.22979500	-1.42852900	-0.94936600
O	2.41212600	0.99738600	-0.24469900
Ni	-0.15781300	-0.03522000	0.41173100

**(1d)**

B	1.11116300	-1.86178000	-0.00405700
B	1.31133000	1.62189300	-0.08077000
B	-1.69274500	1.52666000	-0.08000700
B	-0.23956300	2.21518900	-0.10292900
B	-1.08715200	-1.56523700	-0.08591800
B	-2.19486900	-0.23940200	-0.10635400
B	2.19613400	-0.41683700	0.02290400
O	-0.08307000	-2.47035300	-0.25332300
O	2.24617600	-1.57162300	-0.74892900
O	1.25262100	-0.85735600	1.00784500
O	2.45854600	0.89933600	-0.20375200
O	0.90047200	2.85709700	-0.51447300
O	-2.90819700	0.94406400	-0.19254300
O	-2.41437000	-1.55080600	-0.42728900
Ni	-0.30853300	0.27123900	0.45876300

**(2a)**

B	-1.14334800	1.26861100	0.22205000
B	3.22426200	0.14667500	-0.09792600
B	1.46803600	-1.23315600	0.56986400
B	-0.66657900	-1.57417500	-0.01194100
B	4.81633600	0.38324700	-0.56719500
B	1.18127400	0.96042800	0.73347900
B	-2.70355400	1.77847300	-0.06128200
O	0.04847600	1.73478200	0.51059100
O	0.47749900	-2.14827000	0.13759000
O	0.96864400	-0.23722400	1.37211800
O	-3.78199000	1.30592200	-0.37646700
O	2.68447200	-1.13196100	0.00499800
O	2.37625000	1.21425000	0.15039800
O	5.95285200	0.55411700	-0.90137800
Pd	-2.18895100	-0.41268400	-0.24169700

**(2b)**

B	0.69630700	1.52469800	0.00013300
B	-1.42493100	0.87676200	0.00031600

B	2.61311600	1.25002000	-0.00025400
B	-5.59201700	-0.26785900	-0.00010600
B	-3.14900100	-0.50321700	-0.00057800
B	-0.96325300	-0.74885900	0.00044200
B	1.20114100	-0.18882100	0.00045400
O	1.85654000	2.32716200	-0.00036400
O	-4.42517000	-0.91059000	-0.00133800
O	0.35676700	-1.22886600	0.00083800
O	-0.57023300	1.97397700	0.00022100
O	-2.78235100	0.85388900	-0.00038600
O	-2.11430800	-1.45726100	-0.00008200
O	-6.66513000	0.27737500	0.00104900
Pd	3.21400600	-0.53041600	-0.00003300

**(2c)**

B	1.25209300	1.18912400	-0.00001600
B	-1.06271700	0.48878400	0.00002400
B	2.73145300	1.95521600	-0.00016200
B	-5.40075300	0.50332000	0.00000800
B	-3.11091900	-0.38146800	-0.00009800
B	-1.06436700	-1.21451600	-0.00006200
B	1.15038600	-1.53401200	0.00003800
O	3.91693300	1.66920100	-0.00014000
O	-4.44500000	-0.42756500	-0.00018000
O	0.01072400	-2.12798600	-0.00001200
O	-0.03881100	1.42391300	0.00011700
O	-2.37630800	0.81514900	-0.00007400
O	-2.36128500	-1.57029300	-0.00002200
O	-6.28308900	1.32081500	0.00018500
Pd	2.61171300	-0.30126300	0.00005100

**(2d)**

B	0.97408500	1.14662200	0.00027200
B	-1.43497400	0.68765000	-0.00025900
B	3.06548800	1.54501600	0.00052900
B	-5.26224400	0.32262900	-0.00066900
B	-3.59968600	0.11114900	-0.00021900
B	-1.68127000	-0.99710400	0.00057200
B	0.43935800	-1.52286700	0.00046400
O	3.93705200	0.67702200	-0.00013000
O	-2.70729600	1.18091700	-0.00048900
O	-0.73622500	-2.04560700	0.00095600
O	1.91048500	2.19091300	0.00127600
O	-0.31863100	1.47531700	-0.00039500



O	-3.01603100	-1.17205500	0.00052400
O	-6.44975800	0.47355300	0.00001900
Pd	2.09868400	-0.62404200	-0.00038100

**(3a)**

B	-5.18362300	0.25461100	-0.53561800
B	2.62000100	1.51289500	-0.19424800
B	-1.52768700	0.99205500	0.64219900
B	-3.57792200	0.08059200	-0.08309200
B	0.80479600	1.43614300	0.16707300
B	-1.78766800	-1.22646600	0.63441400
B	0.34129700	-1.62350700	0.08815000
O	1.82566300	2.48750500	0.06948700
O	-0.44938200	1.80566600	0.38274300
O	-1.27019300	-0.16959700	1.33594600
O	-3.01663700	-1.18243600	0.09234900
O	-2.74979200	1.17416800	0.07872300
O	-0.80412100	-2.18125400	0.27215200
O	-6.32969800	0.37873900	-0.85849400
Pt	1.84496500	-0.32864000	-0.18689300

**(3b)**

B	-5.21552100	0.31477300	-0.57108600
B	2.27863900	1.91928100	-0.03598300
B	-1.59684900	1.02073200	0.71733700
B	-3.61778800	0.13085900	-0.09668400
B	0.71787400	1.39103000	0.24151100
B	-1.82677400	-1.19341800	0.59388100
B	0.31512500	-1.49903900	0.05661100
O	3.33990500	1.38063400	-0.32924100
O	-0.49437100	1.83529300	0.49775800
O	-1.34620800	-0.16524100	1.36631600
O	-3.04593300	-1.13200400	0.02921700
O	-2.80148300	1.22603300	0.13311200
O	-0.81851400	-2.10305200	0.19441000
O	-6.35644100	0.44752900	-0.90798400
Pt	1.75526700	-0.28634200	-0.15893100

**(3c)**

B	5.81639700	0.38012500	0.00101000
B	-2.63498700	1.75558900	0.00005000
B	3.51003500	-0.45631200	-0.00045100
B	1.44925500	-1.24794100	-0.00112800
B	-0.81646400	1.32817600	-0.00124100

B	1.47366900	0.45786400	-0.00103100
B	-0.77898100	-1.57893100	-0.00022100
O	-1.62018100	2.54930800	-0.00160200
O	2.80188600	0.74936500	-0.00061600
O	0.36771300	-2.15401200	-0.00159100
O	2.73792300	-1.63097600	-0.00078400
O	4.84478100	-0.53306300	-0.00006800
O	0.50321300	1.43085300	-0.00116100
O	6.71600000	1.17915500	0.00205400
Pt	-2.19109400	-0.20407500	0.00058000

**(3d)**

B	-5.95808600	-0.86155200	-0.00037100
B	2.23449700	1.27608000	-0.00031800
B	-3.81757800	0.33461900	0.00023000
B	-1.90044700	1.42121500	0.00037000
B	0.52589400	-0.03514200	0.00021200
B	-1.69408100	-0.25630500	0.00084300
B	0.29473300	1.72988600	-0.00010900
O	1.55990300	2.39210400	-0.00024200
O	-2.94550000	-0.77426900	0.00056900
O	-0.88305100	2.37266900	-0.00016400
O	-3.24316100	1.61298000	0.00019400
O	-5.15101400	0.19762300	-0.00013000
O	-0.46960100	-0.93573800	0.00055700
O	-6.71478100	-1.79803200	-0.00068500
Pt	2.49170500	-0.54593200	-0.00006500