

Supplementary Information

M₂B₁₀ (M=Rh, Ir): Finally a stable boron-based icosahedral cluster

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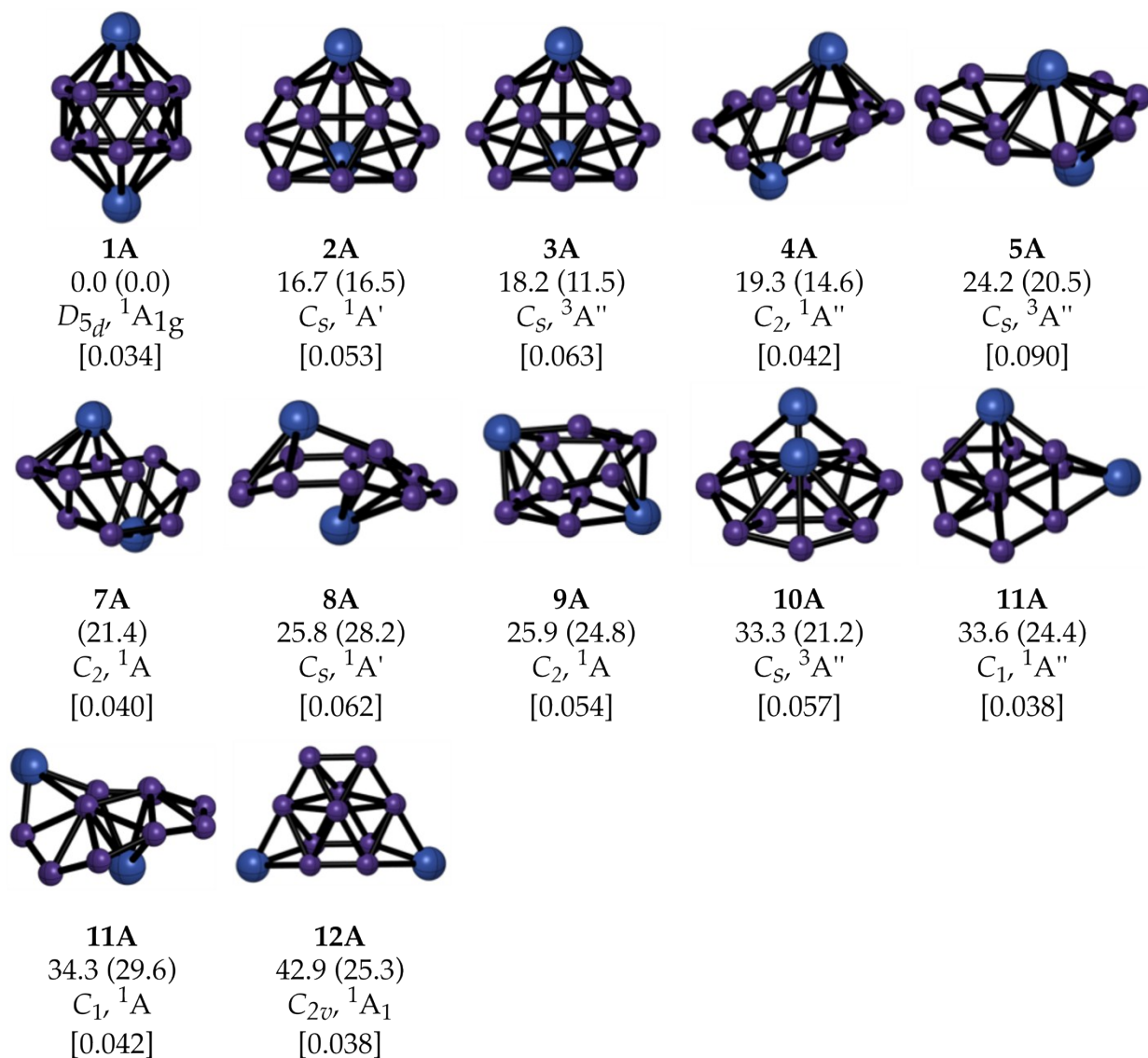


Figure S1. Optimized structures for the lowest-lying energy isomers of the $B_{10}Rh_2$ cluster. Relative energies (in kcal/mol) without parenthesis are computed at the CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level, values in parenthesis are computed at the PBE0/def2-TZVPP level, and values in brackets correspond to the T1 diagnostic analysis.

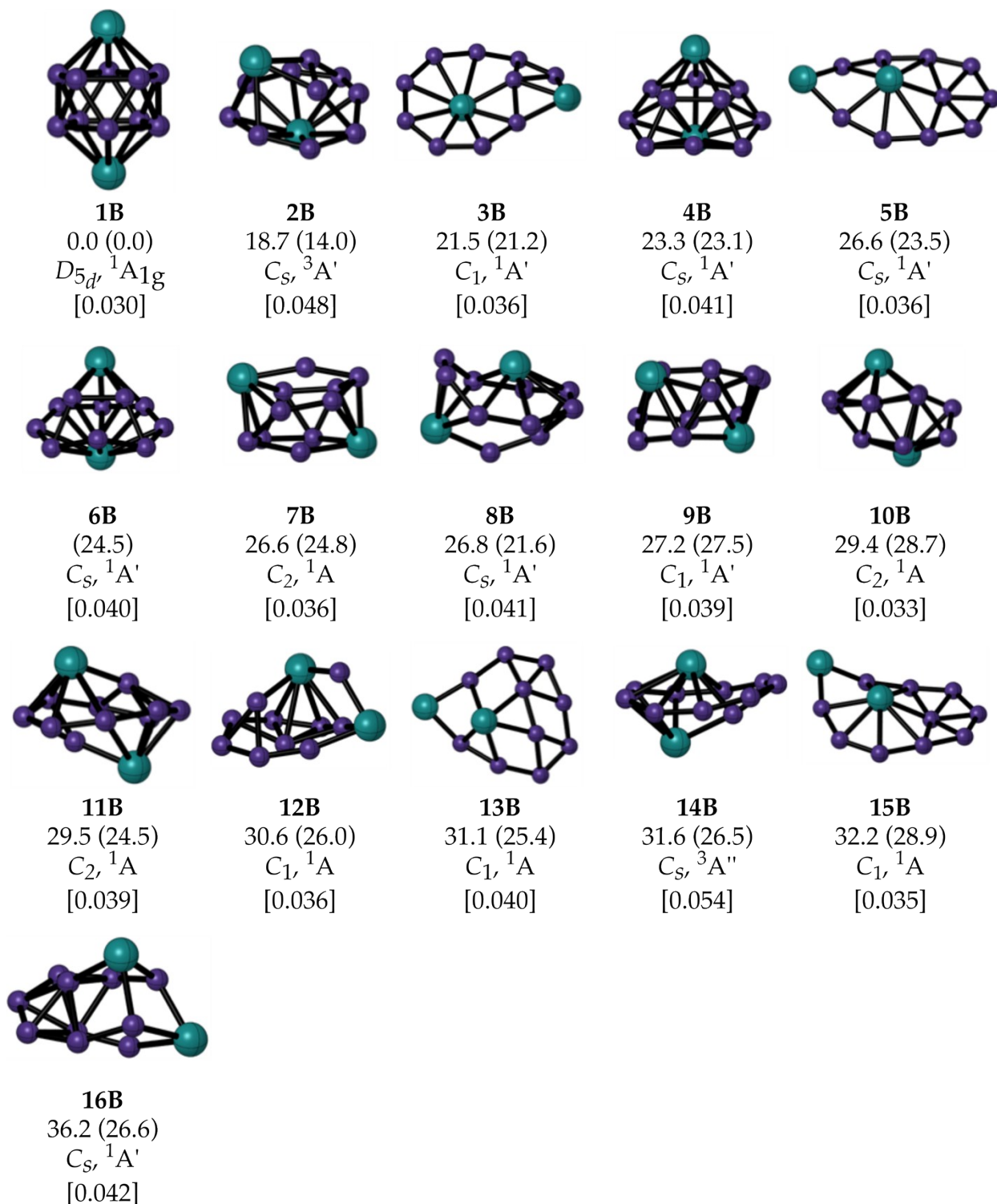


Figure S2. Optimized structures for the lowest-lying energy isomers of the $B_{10}Ir_2$ cluster. Relative energies (in kcal/mol) without parenthesis are computed at the CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level, values in parenthesis are computed at the PBE0/def2-TZVPP level, and values in brackets correspond to the T1 diagnostic analysis.

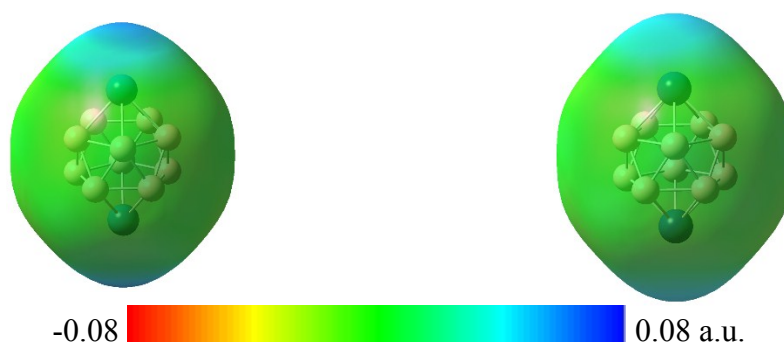


Figure S3. Projection of the electrostatic potential on the molecular van der Waals surface of $B_{10}Rh_2$ (left) and $B_{10}Ir_2$ (right) at the PBE0/def2-TZVPP level. The vdW surface is defined by the $0.001e/\text{bohr}^3$ contour of the electronic density.

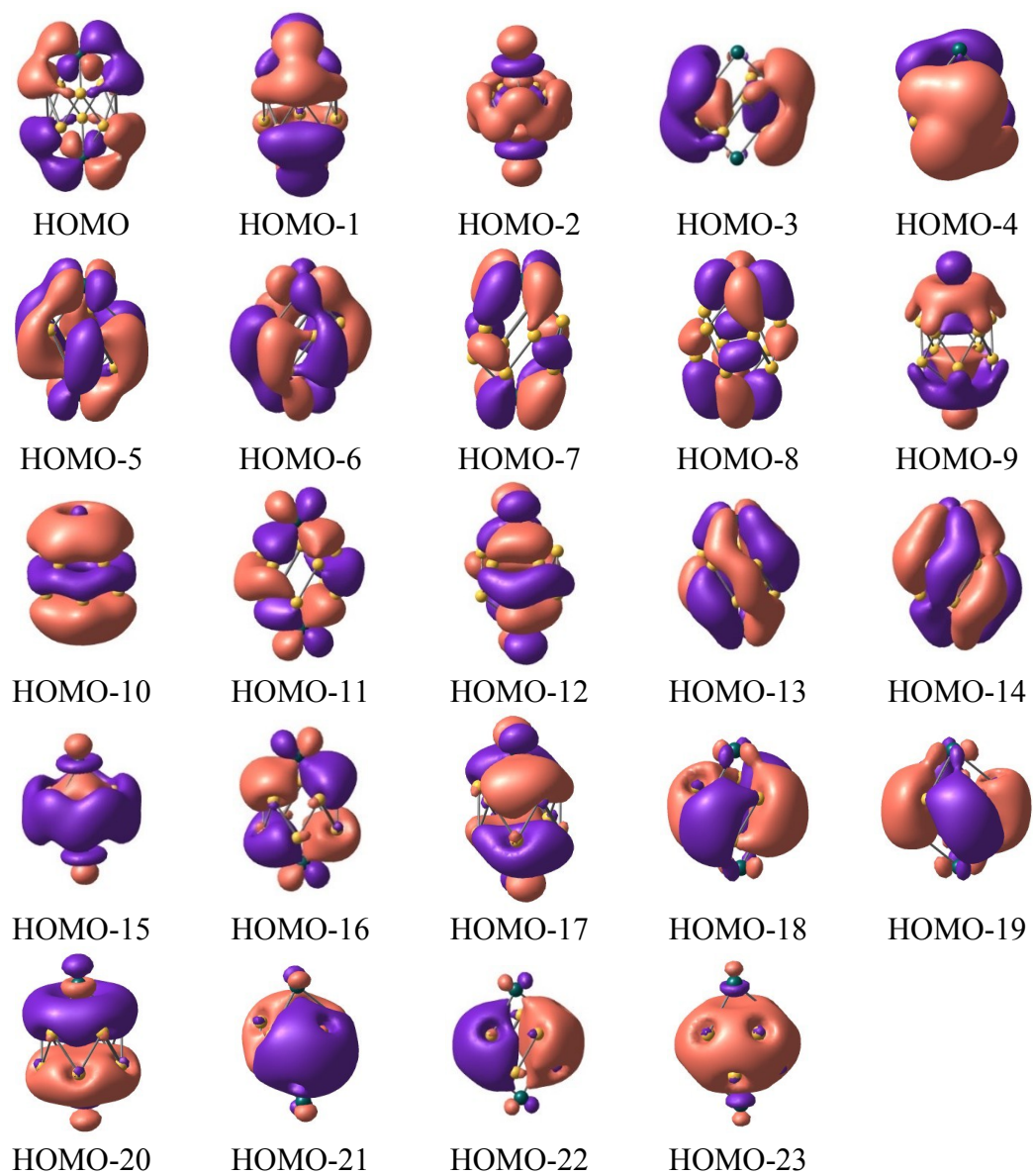


Figure S4. Molecular orbitals of $B_{10}Rh_2$ at the PBE0/def2-TZVPP level.

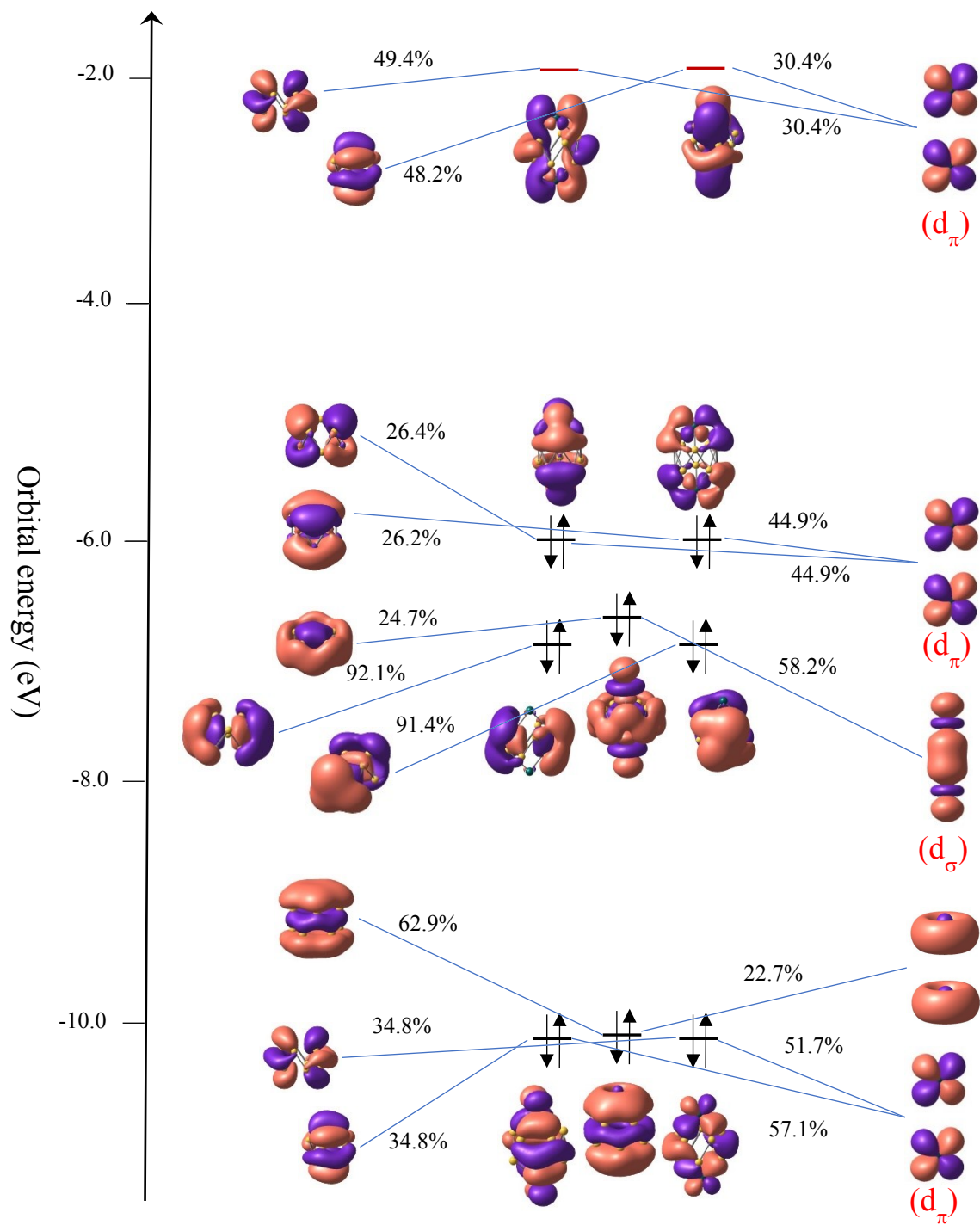


Figure S5. Diagram of orbital interactions between the tubular B₁₀ disk (left) and Rh₂ dimer (right), orbital energy for the complex.

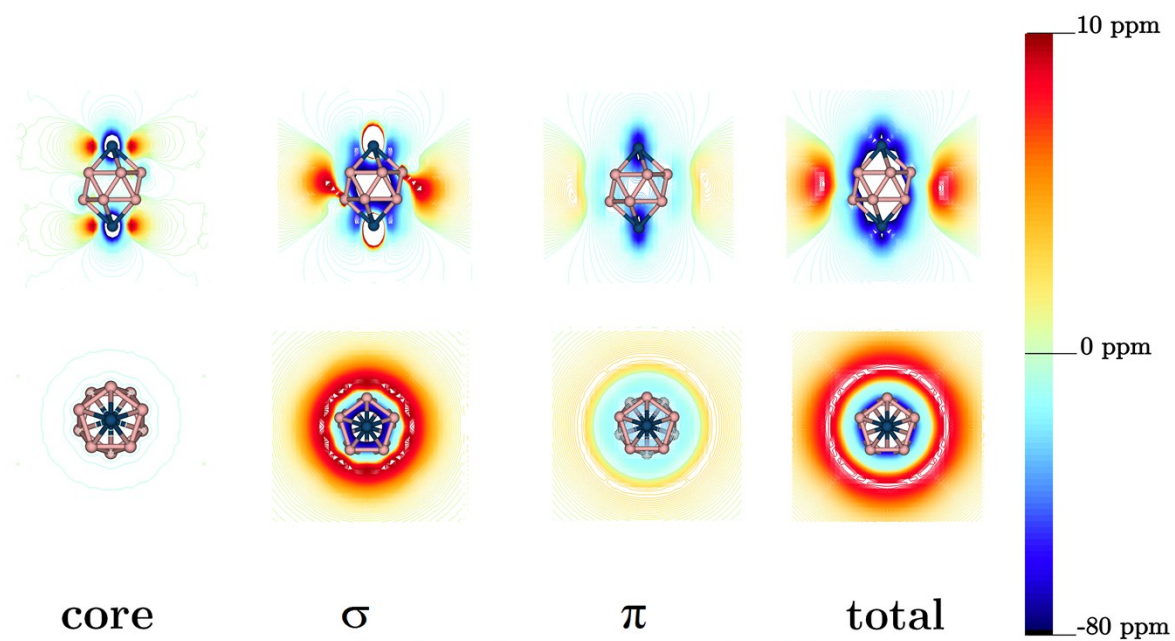


Figure S6. Isolines of the B_z^{ind} for $B_{10}\text{Ir}_2$ computed at PW91/def2-TZVP level. Negative and paratropic values are in blue and red, respectively.

Table S1. Cartesian Coordinates for the six lowest energy structures (see Figure 2) computed at the PBE0/def2-TZVPP level.

B₁₀Rh₂

Rh01

CCSD(T)=-467.9872571 a.u.

B	0.000000000	-1.470819000	0.699730000
B	0.000000000	1.470819000	-0.699730000
B	-0.864525000	-1.189917000	-0.699730000
B	1.398832000	-0.454508000	0.699730000
B	0.864525000	-1.189917000	-0.699730000
B	-1.398832000	-0.454508000	0.699730000
B	0.864525000	1.189917000	0.699730000
B	-1.398832000	0.454508000	-0.699730000
B	-0.864525000	1.189917000	0.699730000
B	1.398832000	0.454508000	-0.699730000
Rh	0.000000000	0.000000000	-2.116566000
Rh	0.000000000	0.000000000	2.116566000

Rh02 (16)

CCSD(T)=-467.9574391 a.u.

B	1.311759000	1.384881000	1.578583000
B	-1.550590000	-0.571034000	0.000000000
B	1.311759000	1.384881000	-1.578583000
B	0.985100000	-0.124769000	0.861532000
B	-0.897532000	-0.322038000	1.454221000
B	-0.897532000	-0.322038000	-1.454221000
B	0.985100000	-0.124769000	-0.861532000
B	0.156121000	0.597634000	-2.216669000
B	1.697983000	1.298232000	0.000000000
B	0.156121000	0.597634000	2.216669000
Rh	0.105782000	-1.747065000	0.000000000
Rh	-0.467814000	1.324997000	0.000000000

Rh03 (16-3t)

CCSD(T)=-467.9556815 a.u.

B	1.282613000	1.390810000	1.546250000
B	-1.646618000	-0.646221000	0.000000000
B	1.282613000	1.390810000	-1.546250000
B	1.083179000	-0.142426000	0.842743000
B	-0.959298000	-0.387343000	1.412572000
B	-0.959298000	-0.387343000	-1.412572000
B	1.083179000	-0.142426000	-0.842743000
B	0.112014000	0.560932000	-2.127715000
B	1.747871000	1.293413000	0.000000000
B	0.112014000	0.560932000	2.127715000
Rh	0.120183000	-1.714538000	0.000000000
Rh	-0.468880000	1.326634000	0.000000000

Rh04 (90)

CCSD(T)=-467.9531935 a.u.

B	1.282613000	1.390810000	1.546250000
B	-1.646618000	-0.646221000	0.000000000
B	1.282613000	1.390810000	-1.546250000
B	1.083179000	-0.142426000	0.842743000
B	-0.959298000	-0.387343000	1.412572000
B	-0.959298000	-0.387343000	-1.412572000
B	1.083179000	-0.142426000	-0.842743000
B	0.112014000	0.560932000	-2.127715000
B	1.747871000	1.293413000	0.000000000
B	0.112014000	0.560932000	2.127715000
Rh	0.120183000	-1.714538000	0.000000000
Rh	-0.468880000	1.326634000	0.000000000

Rh05 (69)

CCSD(T)=-467.9520303 a.u.

B	-0.294487000	2.305587000	1.578845000
B	-0.294487000	-0.443664000	1.431602000
B	-0.117266000	0.917048000	-2.259728000
B	-0.294487000	2.305587000	-1.578845000
B	-0.510362000	2.584949000	0.000000000
B	-1.230553000	-0.345593000	0.000000000
B	-1.196836000	1.039969000	-0.892680000
B	-1.196836000	1.039969000	0.892680000
B	-0.117266000	0.917048000	2.259728000
B	-0.294487000	-0.443664000	-1.431602000
Rh	-0.132138000	-1.951958000	0.000000000
Rh	0.748478000	0.854487000	0.000000000

Rh06 (23)

CCSD(T)=-467.9507239 a.u.

B	1.417214000	1.482920000	1.053551000
B	0.279583000	-1.154948000	0.946192000
B	0.895269000	0.164641000	1.767159000
B	-0.827504000	-1.815928000	-0.353290000
B	-0.279029000	1.154479000	0.945577000
B	-1.416647000	-1.483229000	1.052746000
B	-0.175945000	-0.770122000	-1.368190000
B	-0.894851000	-0.165140000	1.766897000
B	0.175634000	0.771581000	-1.367027000
B	0.828812000	1.816631000	-0.352426000
Rh	1.660756000	-0.238619000	-0.227451000
Rh	-1.661037000	0.238520000	-0.227126000

B₁₀Ir₂

Ir01

CCSD(T)=-455.9458228 a.u.

B	0.000000000	1.494134000	0.700882000
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B	0.000000000	-1.494134000	-0.700882000
B	0.878230000	1.208780000	-0.700882000
B	-1.421006000	0.461713000	0.700882000
B	-0.878230000	1.208780000	-0.700882000
B	1.421006000	0.461713000	0.700882000
B	-0.878230000	-1.208780000	0.700882000
B	1.421006000	-0.461713000	-0.700882000
B	0.878230000	-1.208780000	0.700882000
B	-1.421006000	-0.461713000	-0.700882000
Ir	0.000000000	0.000000000	-2.086576000
Ir	0.000000000	0.000000000	2.086576000

Ir02 (16-3t)

CCSD(T)=-455.9147133 a.u.

B	1.366227000	1.437019000	-1.544330000
B	-0.439517000	-1.659966000	0.000000000
B	1.366227000	1.437019000	1.544330000
B	-0.180968000	1.173791000	-0.853839000
B	-0.257096000	-0.943457000	-1.421585000
B	-0.257096000	-0.943457000	1.421585000
B	-0.180968000	1.173791000	0.853839000
B	0.628201000	0.200128000	2.118638000
B	1.214374000	1.911114000	0.000000000
B	0.628201000	0.200128000	-2.118638000
Ir	-1.633899000	0.041449000	0.000000000
Ir	1.385823000	-0.298168000	0.000000000

Ir03 (7135)

CCSD(T)=-455.9100939 a.u.

B	9.014123000	10.249259000	9.344264000
B	8.757110000	8.946991000	7.822743000
B	12.515654000	8.138913000	8.813985000
B	11.337275000	7.488474000	8.042096000
B	10.331627000	11.021516000	10.183387000
B	8.019148000	10.300812000	7.974936000
B	12.698600000	9.369673000	9.745965000
B	7.852794000	11.455386000	9.018248000
B	11.800964000	10.474654000	10.361462000
B	9.844306000	7.811078000	7.755071000
Ir	8.612654000	11.811922000	10.704341000
Ir	10.816872000	9.512464000	8.669198000

Ir04 (16)

CCSD(T)=-455.9080571 a.u.

B	1.370096000	1.459417000	-1.581497000
B	-0.420729000	-1.582141000	0.000000000
B	1.370096000	1.459417000	1.581497000
B	-0.143477000	1.056232000	-0.884332000
B	-0.194223000	-0.888337000	-1.451363000

B	-0.194223000	-0.888337000	1.451363000
B	-0.143477000	1.056232000	0.884332000
B	0.686036000	0.224848000	2.201528000
B	1.255730000	1.860713000	0.000000000
B	0.686036000	0.224848000	-2.201528000
Ir	-1.662345000	0.042442000	0.000000000
Ir	1.390005000	-0.295244000	0.000000000

Ir05 (5159)

CCSD(T)=-455.9034196 a.u.

B	3.784704000	0.226024000	-1.399129000
B	0.752733000	0.721947000	1.823654000
B	-0.680600000	0.556785000	-1.156056000
B	3.784704000	0.226024000	1.399129000
B	0.752733000	0.721947000	-1.823654000
B	2.295199000	0.413626000	1.783380000
B	-0.680600000	0.556785000	1.156056000
B	2.795856000	0.370066000	0.000000000
B	2.295199000	0.413626000	-1.783380000
B	4.476189000	0.215646000	0.000000000
Ir	0.834535000	-0.323142000	0.000000000
Ir	-2.072147000	0.034704000	0.000000000

Ir06 (90)

CCSD(T)=-455.8983858 a.u.

B	8.377238000	9.644740000	10.082563000
B	10.269833000	8.773453000	9.042897000
B	8.172523000	7.752641000	8.684022000
B	10.161749000	10.268211000	10.202983000
B	10.221465000	9.391645000	7.448798000
B	8.119888000	8.642189000	11.444523000
B	10.370161000	10.447201000	8.638405000
B	7.561144000	7.912293000	10.159795000
B	9.234205000	8.162715000	7.551990000
B	9.474676000	9.487477000	11.403598000
Ir	9.625435000	7.516675000	10.401274000
Ir	8.266588000	9.947126000	8.149631000