

Theoretical Study on Exohedral Complexes $C_6H_6TMB_{40}$ (TM= Sc-Ni)

Ling Pei¹, Li-Juan Zhang, Da-Zhi Li

Figure S1. Equilibrium geometries of $BzTMB_{40}$ in each configuration. The values given correspond to their relative energies (in eV) with respect to the ground states at the PBE0/6-31G(d), PBE0/6-311+G(d) (in parenthesis) and TPSSh/6-311+G(d) (in square brackets) levels, respectively.

Figure S2. Born-Oppenheimer molecular dynamics (BOMD) of $C_{2v} C_6H_6CrB_{40}$ at 500 K. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

Figure S3. The main NAdO orbitals and eigenvalues of $C_6H_6TMB_{40}$ (TM= Sc-Ni)

Figure S4. The global minimum of CoB_{18}^- and NiB_{40}

Table S1 Structural and energetic properties of $C_6H_6TMB_{40}$ (TM= Sc-Ni)

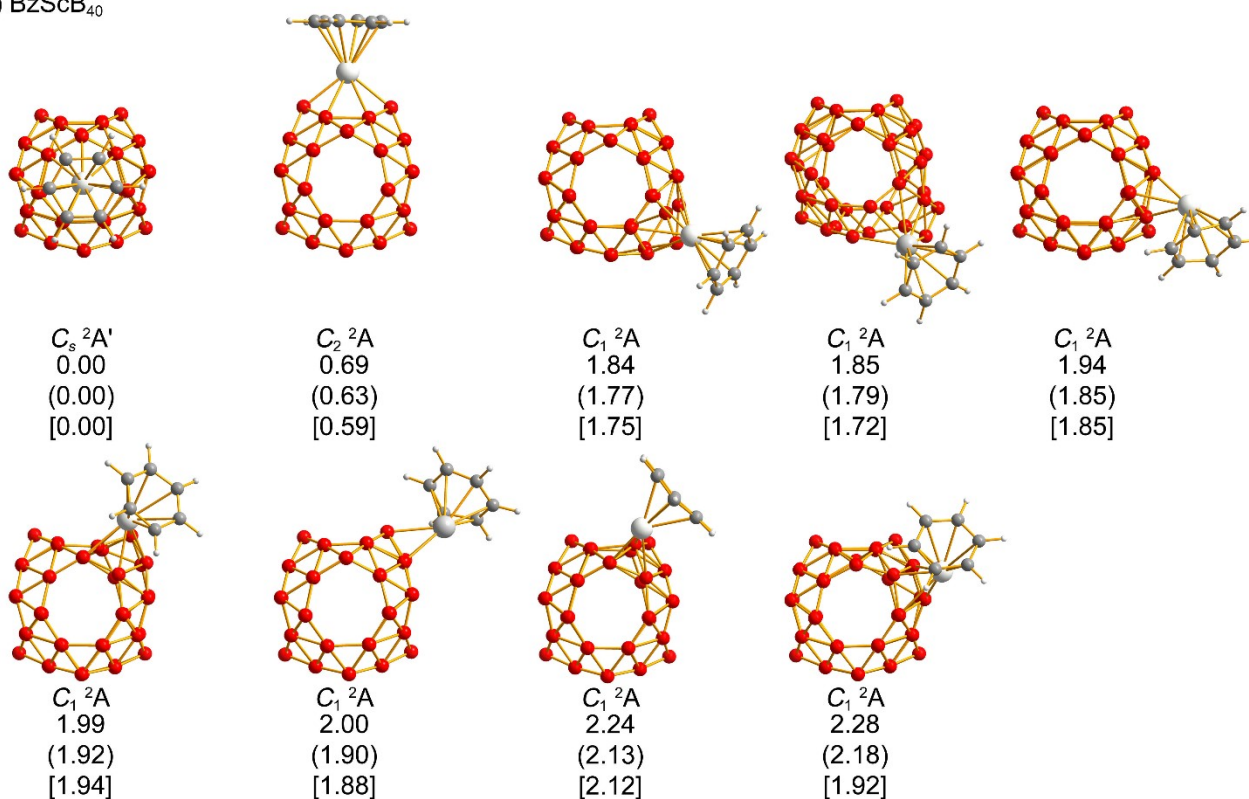
Table S2 Optimized Cartesian coordinates of $C_6H_6TMB_{40}$ (TM= Sc-Ni) at PBE0/6-311+G(d) level

¹ Ling Pei (✉)

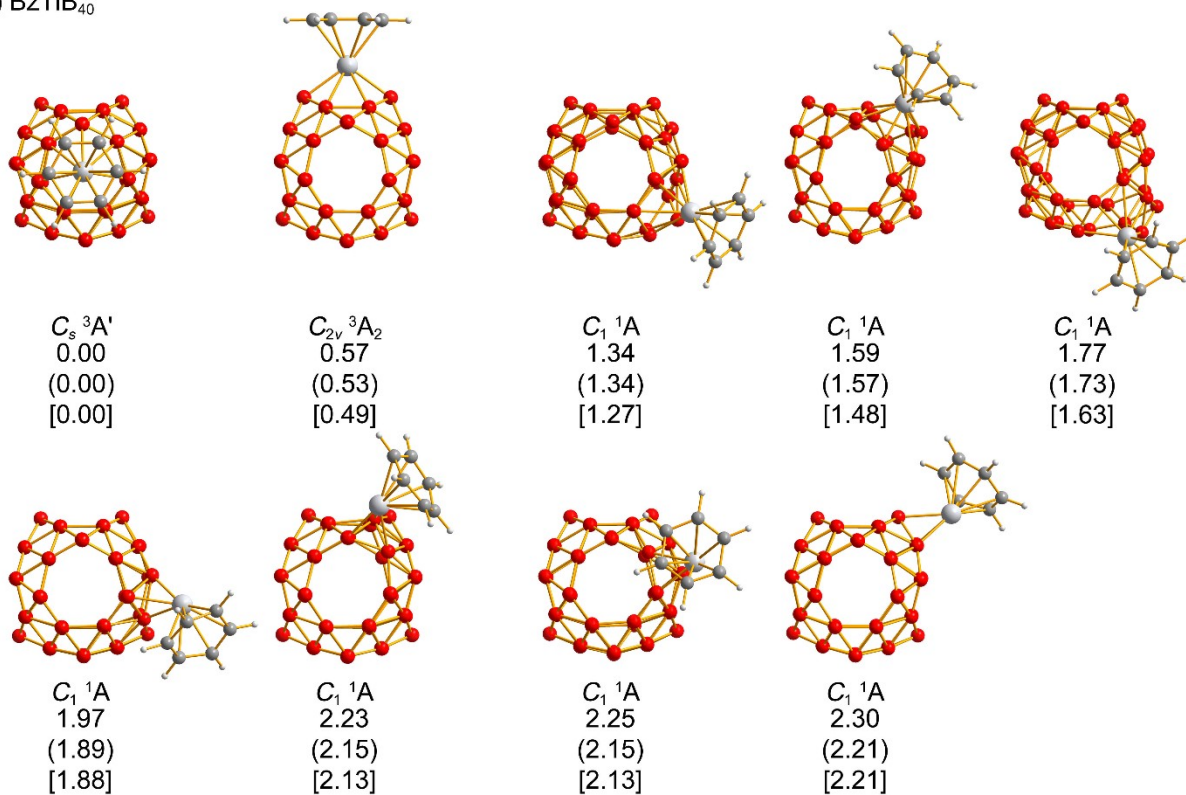
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Figure S1. Equilibrium geometries of BzTMB_{40} in each configuration. The values given correspond to their relative energies (in eV) with respect to the ground states at the PBE0/6-31G(d), PBE0/6-311+G(d) (in parenthesis) and TPSSh/6-311+G(d) (in square brackets) levels, respectively.

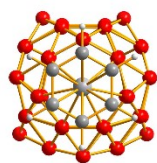
(a) BzScB_{40}



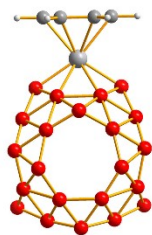
(b) BzTiB_{40}



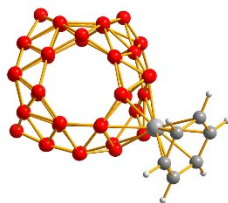
(c) BzVB₄₀



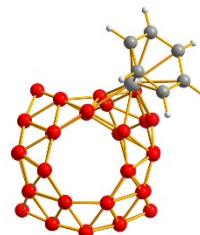
$C_s \ ^2A'$
0.00
(0.00)
[0.00]



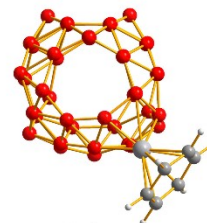
$C_{2v} \ ^2A_1$
0.24
(0.23)
[0.16]



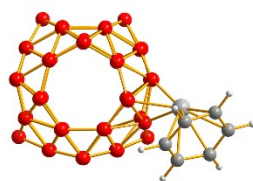
$C_1 \ ^2A$
1.25
(1.25)
[1.17]



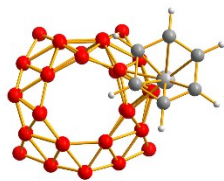
$C_1 \ ^2A$
1.79
(1.75)
[1.68]



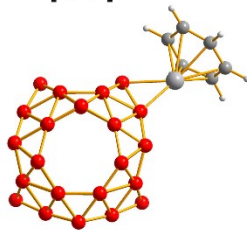
$C_1 \ ^2A$
1.82
(1.77)
[1.70]



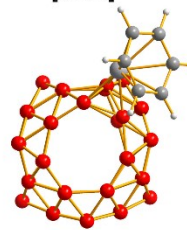
$C_1 \ ^2A$
1.91
(1.80)
[1.81]



$C_1 \ ^2A$
2.11
(1.98)
[1.98]

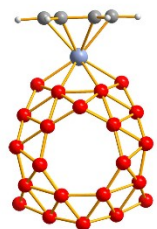


$C_1 \ ^2A$
2.18
(2.06)
[2.09]

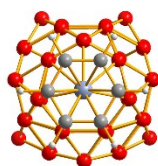


$C_1 \ ^4A$
2.28
(2.12)
[2.31]

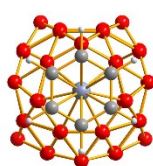
(d) BzCrB₄₀



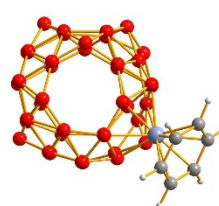
$C_{2v} \ ^1A_1$
0.00
(0.00)
[0.00]



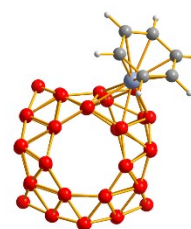
$C_s \ ^1A'$
0.09
(0.06)
[0.12]



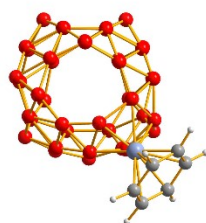
$C_s \ ^1A'$
0.10
(0.06)
[0.13]



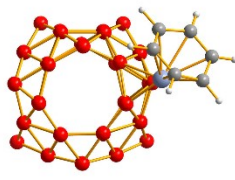
$C_1 \ ^1A$
1.30
(1.33)
[1.32]



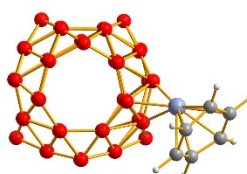
$C_1 \ ^3A$
1.47
(1.49)
[1.75]



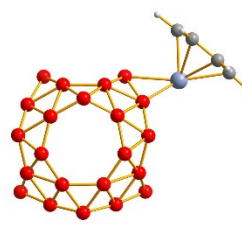
$C_1 \ ^1A$
1.51
(1.55)
[1.52]



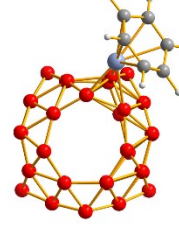
$C_1 \ ^3A$
1.66
(1.58)
[1.99]



$C_1 \ ^3A$
1.66
(1.58)
[1.99]

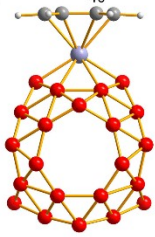


$C_1 \ ^3A$
1.78
(1.73)
[2.13]

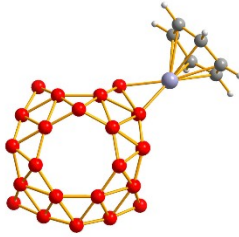


$C_1 \ ^3A$
1.80
(1.71)
[2.12]

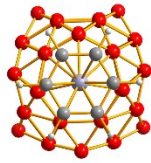
(e) BzMnB_{40}



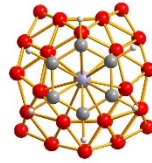
$C_{2v} \ ^2B_1$
0.00
(0.00)
[0.00]



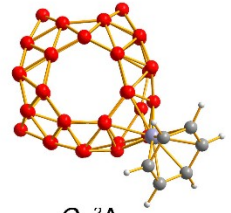
$C_1 \ ^4A$
0.38
(0.28)
[0.99]



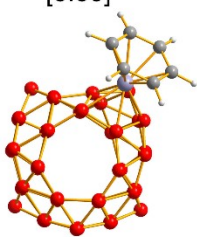
$C_s \ ^2A'$
0.39
(0.35)
[0.39]



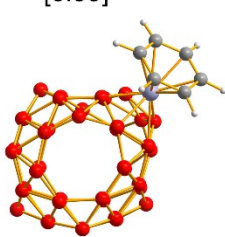
$C_s \ ^2A'$
0.40
(0.36)
[0.40]



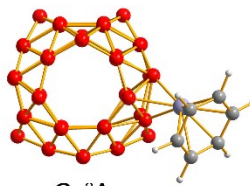
$C_1 \ ^2A$
0.74
(0.83)
[0.83]



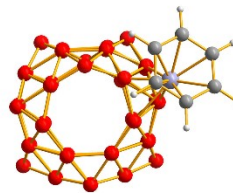
$C_1 \ ^2A$
0.80
(0.93)
[0.89]



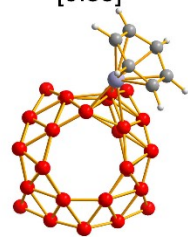
$C_1 \ ^2A$
0.82
(0.91)
[0.87]



$C_1 \ ^2A$
1.05
(1.06)
[1.31]

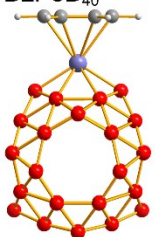


$C_1 \ ^2A$
1.14
(1.07)
[1.29]

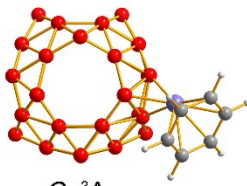


$C_1 \ ^2A$
1.20
(1.18)
[1.42]

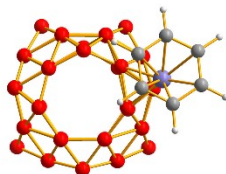
(f) BzFeB_{40}



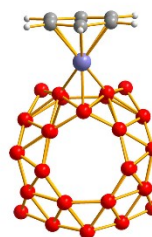
$C_{2v} \ ^3A_2$
0.00
(0.00)
[0.00]



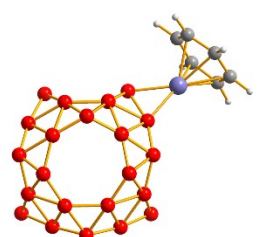
$C_1 \ ^3A$
0.17
(0.27)
[0.29]



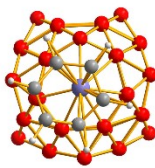
$C_1 \ ^3A$
0.17
(0.25)
[0.27]



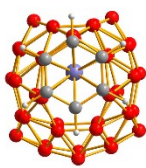
$C_s \ ^3A'$
0.28
(0.37)
[0.40]



$C_s \ ^3A'$
0.30
(0.41)
[0.44]



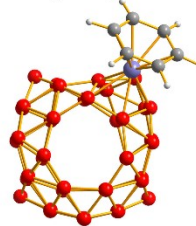
$C_1 \ ^1A$
0.56
(0.72)
[0.28]



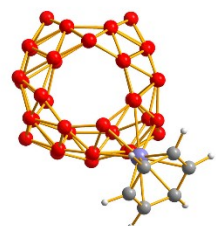
$C_s \ ^1A'$
0.65
(0.82)
[0.27]



$C_1 \ ^1A$
0.71
(0.92)
[0.42]

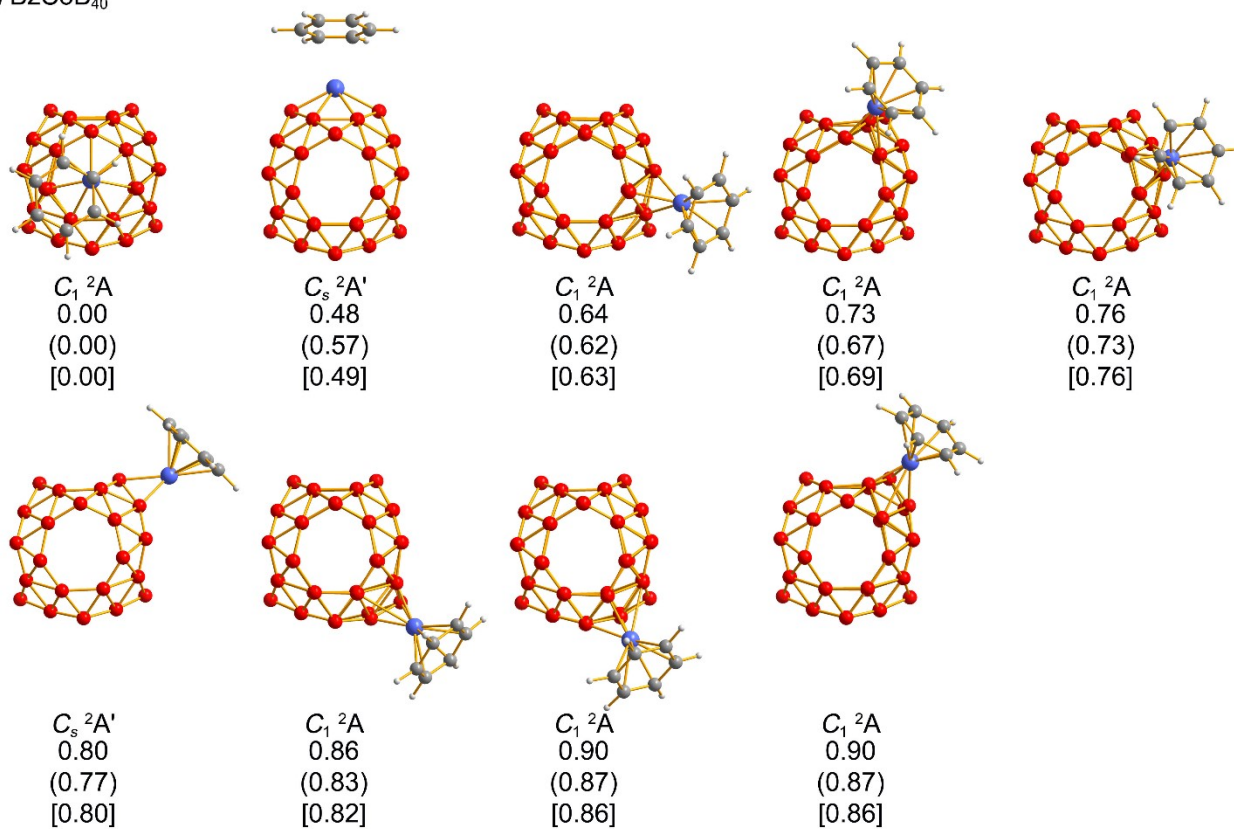


$C_1 \ ^1A$
0.82
(1.08)
[0.56]



$C_1 \ ^1A$
0.89
(1.10)
[0.61]

(g) BzCoB₄₀



(h) BzNiB₄₀

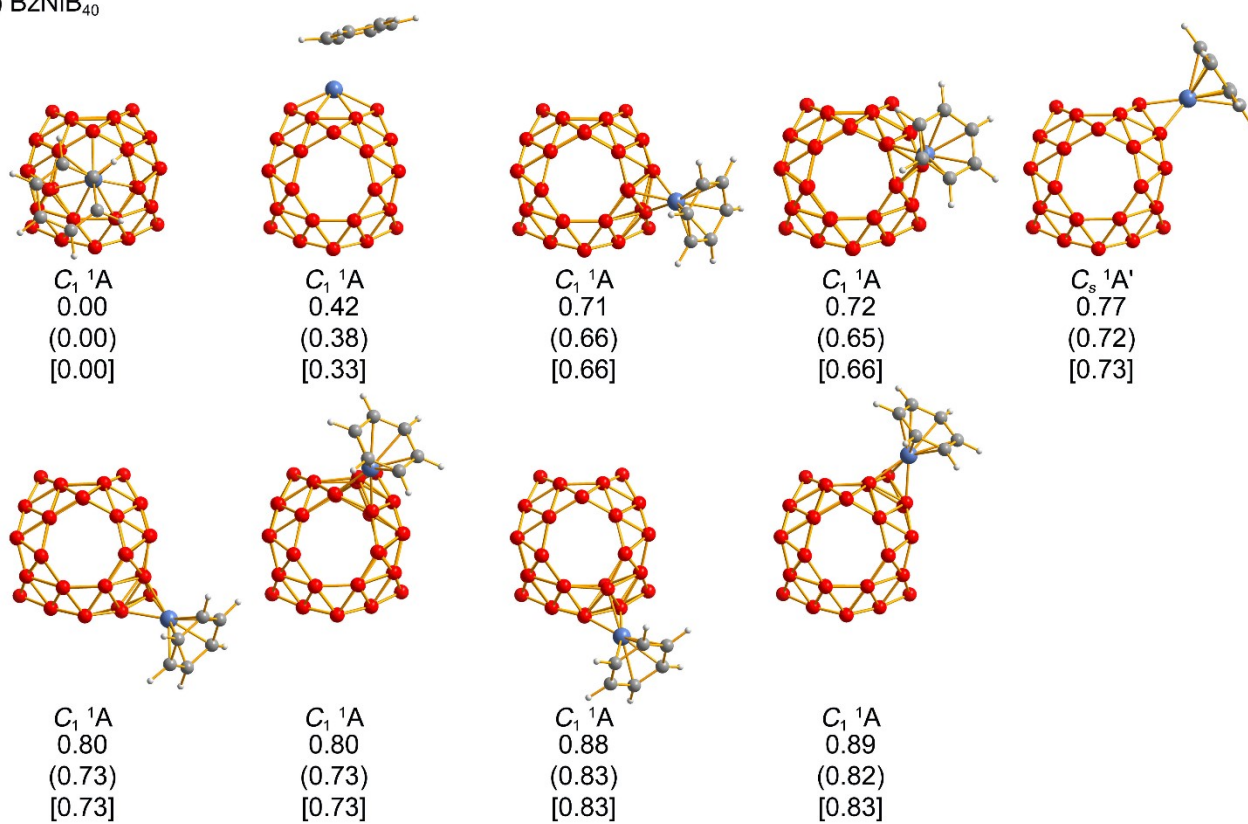


Figure S2. Born-Oppenheimer molecular dynamics (BOMD) of C_{2v} $C_6H_6CrB_{40}$ at 500 K. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

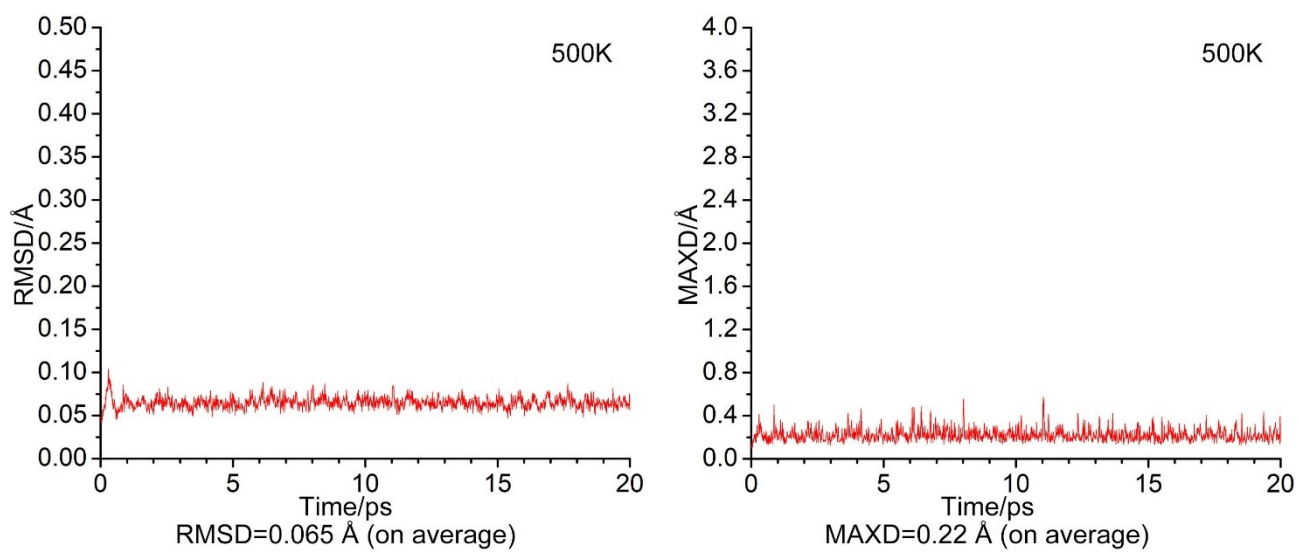
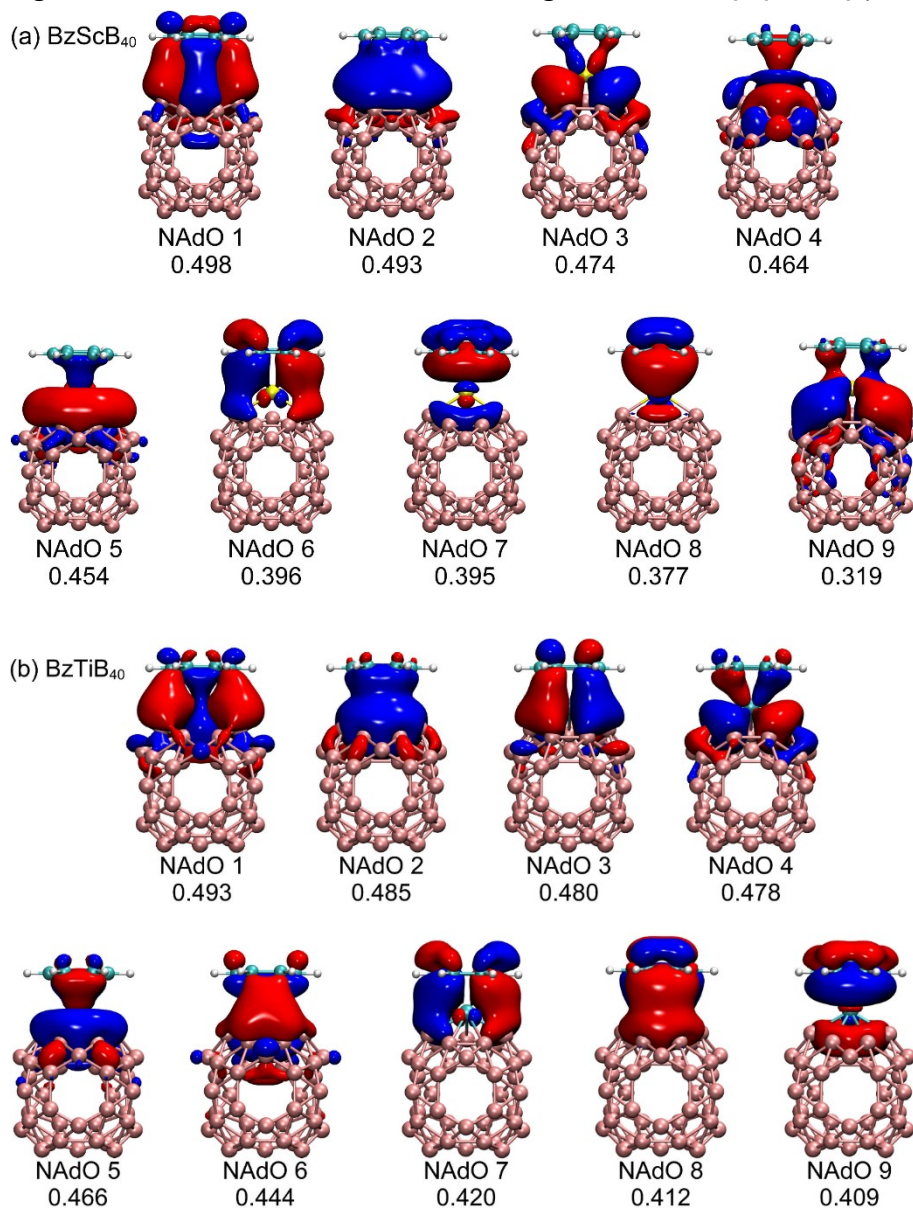
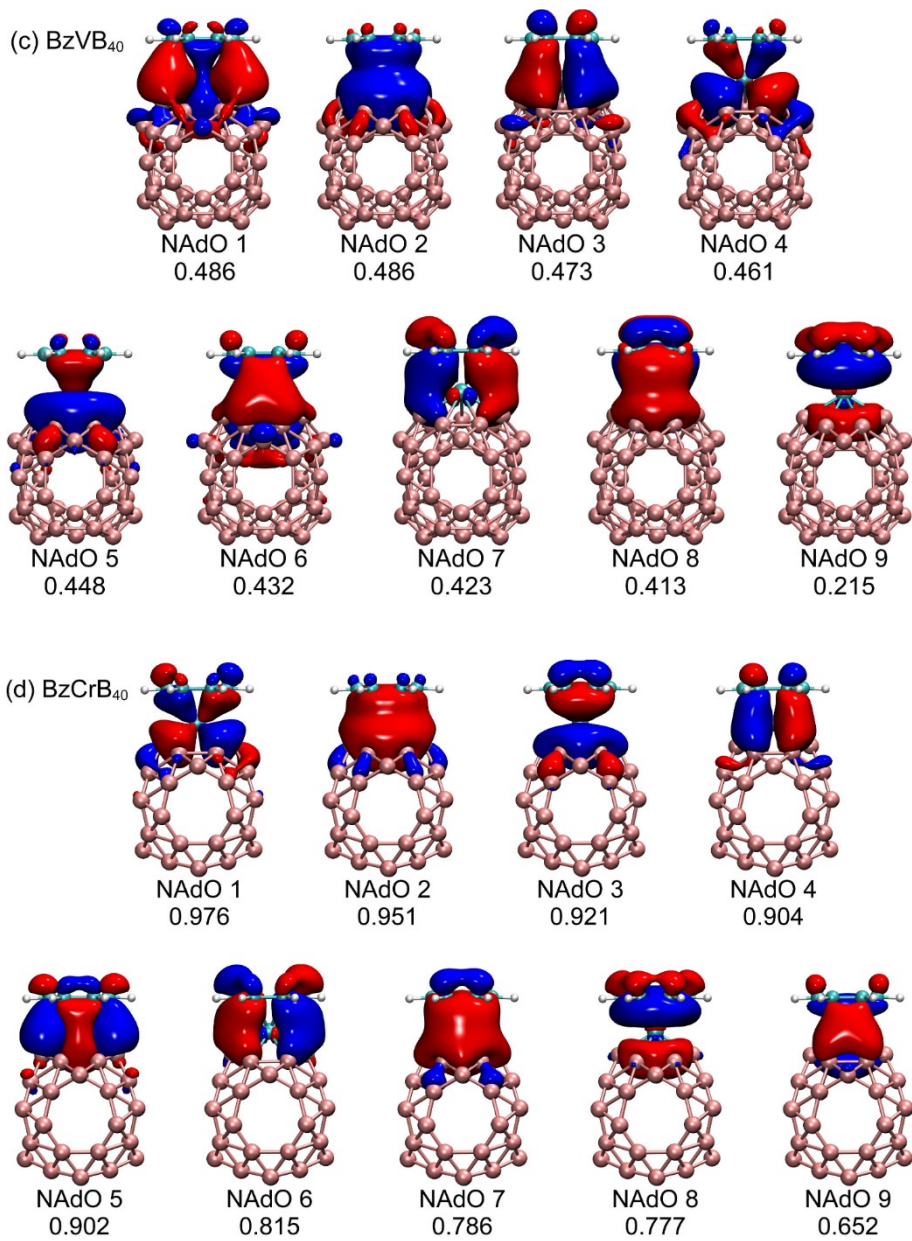
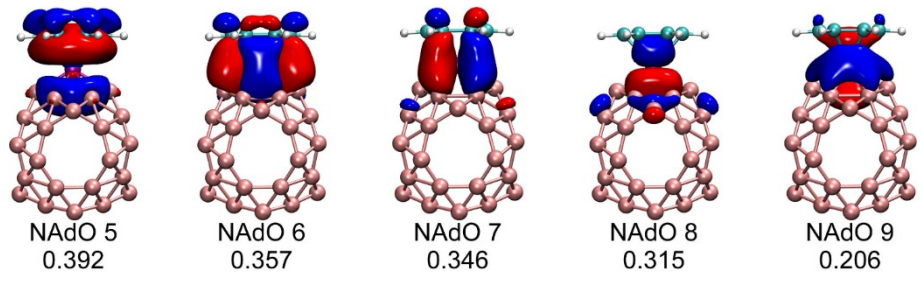
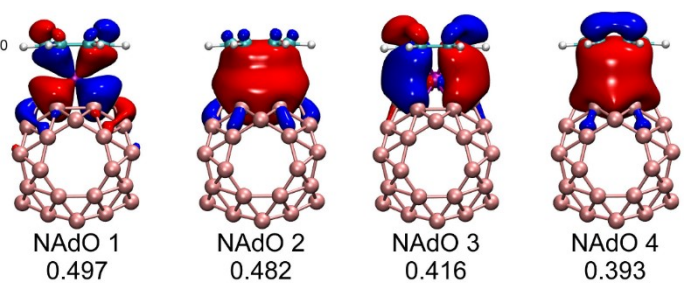


Figure S3. The main NAdO orbitals and eigenvalues of $C_6H_6TM B_{40}$ (TM= Sc-Ni) (isovalue=0.02).

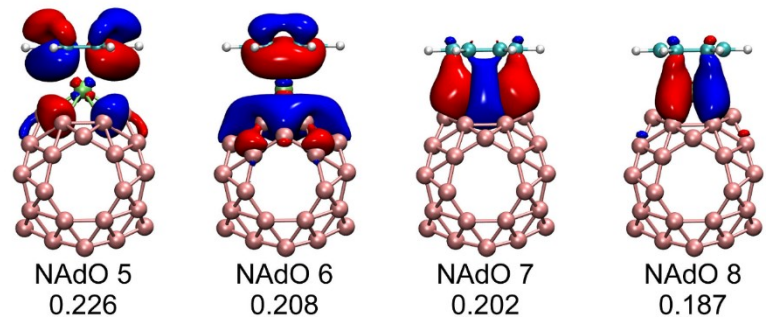
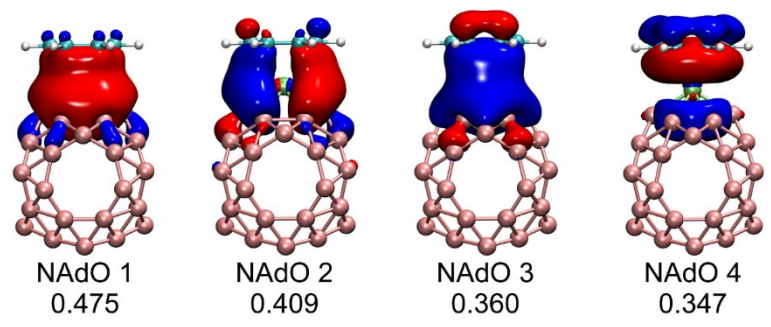




(e) BzMnB₄₀



(f) BzFeB₄₀



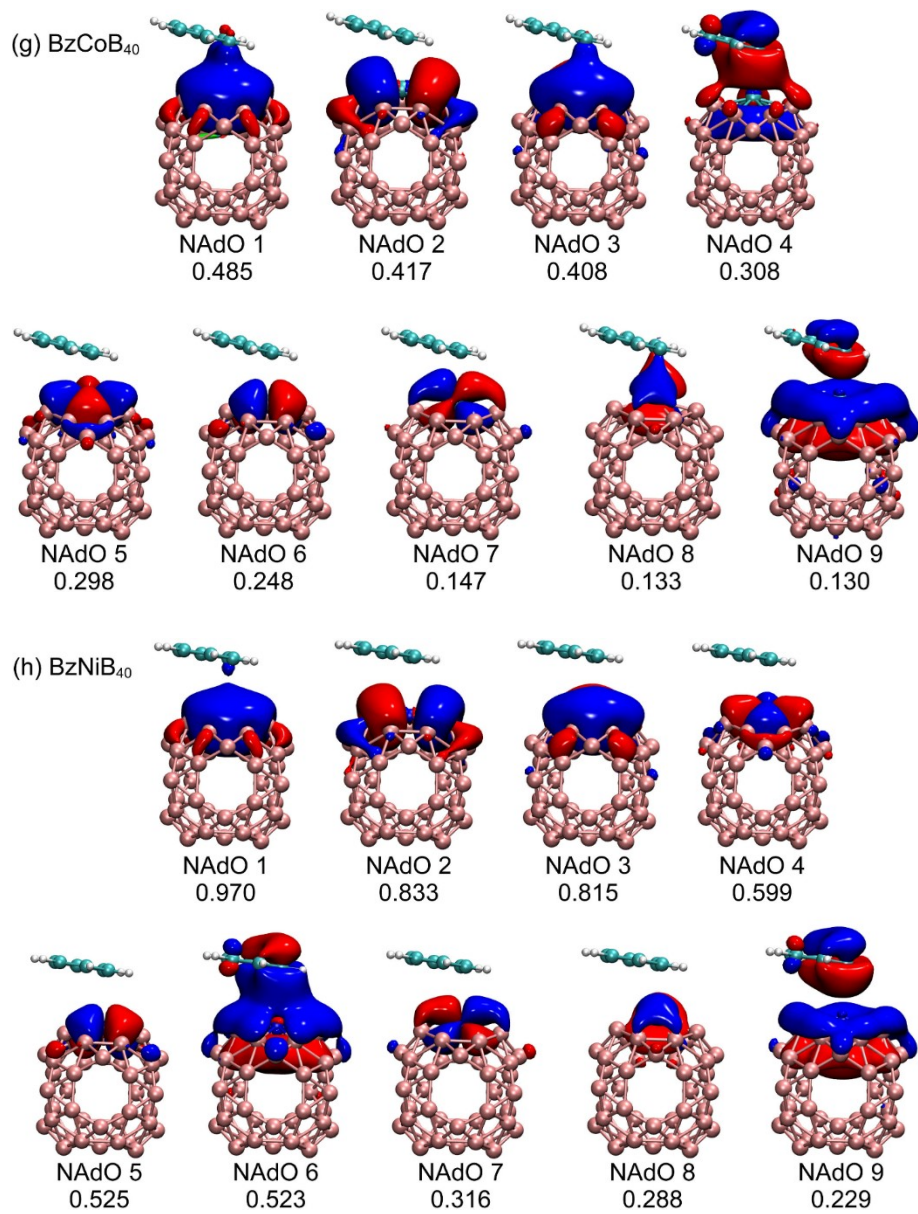


Figure S4. The global minimum of CoB_{18}^- and NiB_{40}

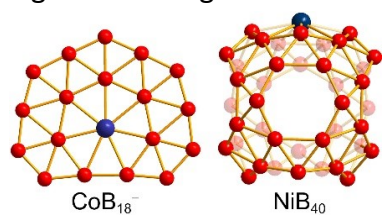


Table S1 Structural and energetic properties of C₆H₆TM_B₄₀ (TM= Sc-Ni)

TM	site	M ^a	PGs ^a	State	R _{TM-B₄₀} ^a	R _{TM-B_z} ^a	E _b	NICS	Δ	Q _{B₄₀}	Q _{TM}	Q _{B_z}	Electron configuration	Mayor	Fuzzy bond order	R _{B-B(B₄₀)} ^b	R _{C-C(B_z)} ^c
1-Sc	η ⁷	2	C _s	² A'	1.53	2.13	5.47	44.89	1.32	-0.98	0.96	0.03	[core]4S(0.17)3d(1.79)	4.40	9.59	1.66-1.69	1.39-1.41
2-Ti	η ⁷	3	C _s	³ A''	1.40	1.89	6.05	38.75	1.63	-0.30	0.23	0.08	[core]4S(0.17)3d(3.48)	5.61	10.02	1.65-1.69	1.40-1.42
3-V	η ⁷	2	C _s	² A'	1.32	1.74	5.31	44.63	2.08	0.07	-0.25	0.18	[core]4S(0.18)3d(4.94)	6.31	10.07	1.65-1.70	1.41-1.43
4-Cr	η ⁶	1	C _{2v}	¹ A ₁	1.34	1.64	3.14	49.29	2.63	0.39	-0.73	0.33	[core]4S(0.20)3d(6.39)	6.84	9.53	1.68-1.78	1.41
5-Mn	η ⁶	2	C _{2v}	² B ₁	1.34	1.66	3.45	43.98	2.13	0.23	-0.56	0.33	[core]4S(0.18)3d(7.26)	5.80	9.26	1.69-1.77	1.41-1.42
6-Fe	η ⁶	3	C _{2v}	³ A ₂	1.36	1.92	3.81	46.05	2.83	-0.23	0.09	0.15	[core]4S(0.15)3d(7.66)	4.49	7.73	1.68-1.80	1.40-1.41
7-Co	η ⁷	2	C ₁	² A	0.85	2.92	3.96	46.04	2.92	-0.48	0.41	0.07	[core]4S(0.15)3d(8.40)	5.18	7.05	1.67-1.75	1.39-1.40
8-Ni	η ⁷	1	C ₁	¹ A	1.08	2.68	4.38	43.78	2.89	-0.47	0.45	0.02	[core]4S(0.16)3d(9.36)	4.84	6.56	1.59-1.76	1.39-1.40

a: Spin multiplicity M, point group symmetry PGs, the distances of TM-B₄₀ and TM-B_z (Å), binding energy E_b (eV), HOMO-LUMO gap Δ (eV)

b: Bond length of B-B in B₄₀ for those B atoms directly bonded to TM.

c: Bond length of C-C in C₆H₆.

Table S2 Optimized Cartesian coordinates of C₆H₆TMB₄₀ (TM= Sc-Ni) at PBE0/6-311+G(d) level

(1) C₆H₆ScB₄₀

B	-0.47518	-4.07762	1.76777
B	2.82066	-1.40992	1.66719
B	1.11242	-3.75077	1.37212
B	-0.30078	1.53782	-1.88255
B	-2.81496	0.45976	0.00000
B	-1.96398	-1.25808	2.59906
B	1.68413	-0.48858	-2.37272
B	-1.22544	-2.67375	-2.34807
B	-0.47518	-4.07762	-1.76777
B	2.82066	-1.40992	-1.66719
B	1.11242	-3.75077	-1.37212
B	0.45000	0.41583	2.78670
B	1.24749	1.03161	1.43518
B	1.24749	1.03161	-1.43518
B	-1.53991	1.10359	-0.84491
B	-1.74338	-3.66628	0.87759
B	1.64853	-2.26692	-2.37026
B	-1.53991	1.10359	0.84491
B	2.01798	1.33368	0.00000
B	0.33170	-3.09613	2.72478
B	1.64853	-2.26692	2.37026
B	1.68413	-0.48858	2.37272
B	-1.10970	0.10100	-2.33872
B	-1.22544	-2.67375	2.34807
B	-1.10970	0.10100	2.33872
B	2.49978	-0.01649	-0.85517
B	2.49978	-0.01649	0.85517
B	-0.30078	1.53782	1.88255
B	-2.49123	-0.34191	1.37379
B	-1.96398	-1.25808	-2.59906
B	-1.74338	-3.66628	-0.87759
B	2.46376	-2.79393	-0.87609
B	2.46376	-2.79393	0.87609
B	-2.53421	-2.13447	1.36146
B	0.45000	0.41583	-2.78670
B	1.90123	-4.05914	0.00000
B	-2.49123	-0.34191	-1.37379
B	-2.90764	-2.95215	0.00000
B	0.33170	-3.09613	-2.72478
B	-2.53421	-2.13447	-1.36146
C	-0.03022	4.85504	-1.40972
C	1.18067	4.96575	-0.69684

C	1.18067	4.96575	0.69684
C	-0.03022	4.85504	1.40972
C	-1.24999	4.87127	0.69335
C	-1.24999	4.87127	-0.69335
H	-0.03176	4.84668	-2.49226
H	2.12209	5.00837	-1.23391
H	2.12209	5.00837	1.23391
H	-0.03176	4.84668	2.49226
H	-2.18964	4.83475	1.23380
H	-2.18964	4.83475	-1.23380
Sc	0.07921	2.77405	0.00000

(2) C₆H₆TiB₄₀

B	-0.41965800	-4.00997200	1.75371600
B	2.82794400	-1.29181700	1.66985600
B	1.17511600	-3.66238800	1.39385800
B	-0.34561500	1.57448100	-1.87206000
B	-2.82691700	0.44824600	0.00000000
B	-1.95099300	-1.23349200	2.61242700
B	1.66191000	-0.42735500	-2.38620700
B	-1.21596000	-2.65038700	-2.37108800
B	-0.41965800	-4.00997200	-1.75371600
B	2.82794400	-1.29181700	-1.66985600
B	1.17511600	-3.66238800	-1.39385800
B	0.41684100	0.48347900	2.77910000
B	1.20843600	1.13628500	1.43870300
B	1.20843600	1.13628500	-1.43870300
B	-1.59163500	1.13675700	-0.84643700
B	-1.70722700	-3.63036600	0.88150100
B	1.66655800	-2.18255700	-2.36616000
B	-1.59163500	1.13675700	0.84643700
B	1.97013800	1.39703000	0.00000000
B	0.36074500	-3.02888100	2.72938000
B	1.66655800	-2.18255700	2.36616000
B	1.66191000	-0.42735500	2.38620700
B	-1.15200200	0.16164700	-2.34972900
B	-1.21596000	-2.65038700	2.37108800
B	-1.15200200	0.16164700	2.34972900
B	2.47468400	0.09647400	-0.87066100
B	2.47468400	0.09647400	0.87066100
B	-0.34561500	1.57448100	1.87206000
B	-2.49986600	-0.35018700	1.37713000
B	-1.95099300	-1.23349200	-2.61242700
B	-1.70722700	-3.63036600	-0.88150100

B	2.50764600	-2.68724200	-0.88098000
B	2.50764600	-2.68724200	0.88098000
B	-2.52873200	-2.13198600	1.39091300
B	0.41684100	0.48347900	-2.77910000
B	1.94153400	-3.94029200	0.00000000
B	-2.49986600	-0.35018700	-1.37713000
B	-2.86793000	-2.91905200	0.00000000
B	0.36074500	-3.02888100	-2.72938000
B	-2.52873200	-2.13198600	-1.39091300
C	-1.22676200	4.59808400	-0.69945800
C	-0.00238500	4.57190100	-1.41067600
C	1.21491700	4.60105900	-0.70566500
C	1.21491700	4.60105900	0.70566500
C	-0.00238500	4.57190100	1.41067600
C	-1.22676200	4.59808400	0.69945800
H	-2.16473100	4.57280500	-1.24204900
H	-0.00520200	4.56597800	-2.49385900
H	2.15506500	4.58816700	-1.24471600
H	2.15506500	4.58816700	1.24471600
H	-0.00520200	4.56597800	2.49385900
H	-2.16473100	4.57280500	1.24204900
Ti	0.01065700	2.69722500	0.00000000

(3) C₆H₆VB₄₀

B	-0.37271800	-3.96881100	1.74017200
B	2.83003900	-1.21019500	1.66781000
B	1.23276500	-3.60939900	1.41872800
B	-0.38952100	1.58906900	-1.85585800
B	-2.83789300	0.42121600	0.00000000
B	-1.92977400	-1.22665800	2.61800300
B	1.64879700	-0.40056300	-2.40278800
B	-1.20884600	-2.65170600	-2.39387700
B	-0.37271800	-3.96881100	-1.74017200
B	2.83003900	-1.21019500	-1.66781000
B	1.23276500	-3.60939900	-1.41872800
B	0.39285700	0.52014100	2.74984300
B	1.17796500	1.23124300	1.42813200
B	1.17796500	1.23124300	-1.42813200
B	-1.63979900	1.13948100	-0.84941700
B	-1.67901500	-3.62011700	0.88802900
B	1.68557900	-2.13746700	-2.36382300
B	-1.63979900	1.13948100	0.84941700
B	1.96096200	1.44716700	0.00000000
B	0.38542500	-2.98981200	2.73312400

B	1.68557900	-2.13746700	2.36382300
B	1.64879700	-0.40056300	2.40278800
B	-1.19408700	0.20629700	-2.34568800
B	-1.20884600	-2.65170600	2.39387700
B	-1.19408700	0.20629700	2.34568800
B	2.45086200	0.17681100	-0.88773400
B	2.45086200	0.17681100	0.88773400
B	-0.38952100	1.58906900	1.85585800
B	-2.51205700	-0.38440400	1.37723700
B	-1.92977400	-1.22665800	-2.61800300
B	-1.67901500	-3.62011700	-0.88802900
B	2.54599400	-2.62017400	-0.88538000
B	2.54599400	-2.62017400	0.88538000
B	-2.52081100	-2.15144200	1.41554400
B	0.39285700	0.52014100	-2.74984300
B	1.96867000	-3.85995600	0.00000000
B	-2.51205700	-0.38440400	-1.37723700
B	-2.83233400	-2.90848400	0.00000000
B	0.38542500	-2.98981200	-2.73312400
B	-2.52081100	-2.15144200	-1.41554400
C	-0.72081400	4.36800200	-1.22112200
C	0.70261600	4.40088600	-1.22055700
C	1.39713900	4.44990400	0.00000000
C	0.70261600	4.40088600	1.22055700
C	-0.72081400	4.36800200	1.22112200
C	-1.42365300	4.38954600	0.00000000
H	-1.26112100	4.34705200	-2.15972700
H	1.24582700	4.37112300	-2.15723100
H	2.48150200	4.43458800	0.00000000
H	1.24582700	4.37112300	2.15723100
H	-1.26112100	4.34705200	2.15972700
H	-2.50624500	4.33158900	0.00000000
V	0.00431400	2.65702000	0.00000000

(4) $C_6H_6CrB_{40}$

B	-2.72357300	1.73871100	-1.65911500
B	0.00000000	1.75090200	1.66520200
B	-2.33805700	1.37538500	-0.06566500
B	2.72357300	-1.73871100	-1.65911500
B	1.68418500	0.00000000	-4.14192400
B	0.00000000	2.62992800	-3.24925600
B	0.86674600	-2.33759600	0.41899100
B	-1.39823900	-2.36312000	-2.48471300
B	-2.72357300	-1.73871100	-1.65911500

B	0.00000000	-1.75090200	1.66520200
B	-2.33805700	-1.37538500	-0.06566500
B	1.72294200	2.69541400	-0.88988200
B	2.33805700	1.37538500	-0.06566500
B	2.33805700	-1.37538500	-0.06566500
B	2.36460900	-0.87644400	-2.95413700
B	-2.36460900	0.87644400	-2.95413700
B	-0.86674600	-2.33759600	0.41899100
B	2.36460900	0.87644400	-2.95413700
B	2.64289400	0.00000000	0.70912700
B	-1.72294200	2.69541400	-0.88988200
B	-0.86674600	2.33759600	0.41899100
B	0.86674600	2.33759600	0.41899100
B	1.39823900	-2.36312000	-2.48471300
B	-1.39823900	2.36312000	-2.48471300
B	1.39823900	2.36312000	-2.48471300
B	1.40420200	-0.88773900	1.33870600
B	1.40420200	0.88773900	1.33870600
B	2.72357300	1.73871100	-1.65911500
B	0.88674500	1.39022100	-3.81797000
B	0.00000000	-2.62992800	-3.24925600
B	-2.36460900	-0.87644400	-2.95413700
B	-1.40420200	-0.88773900	1.33870600
B	-1.40420200	0.88773900	1.33870600
B	-0.88674500	1.39022100	-3.81797000
B	1.72294200	-2.69541400	-0.88988200
B	-2.64289400	0.00000000	0.70912700
B	0.88674500	-1.39022100	-3.81797000
B	-1.68418500	0.00000000	-4.14192400
B	-1.72294200	-2.69541400	-0.88988200
B	-0.88674500	-1.39022100	-3.81797000
Cr	0.00000000	0.00000000	2.78476000
C	1.22551600	-0.70417800	4.42341800
C	0.00000000	-1.40630200	4.43210000
C	-1.22551600	-0.70417800	4.42341800
C	-1.22551600	0.70417800	4.42341800
C	0.00000000	1.40630200	4.43210000
C	1.22551600	0.70417800	4.42341800
H	2.16221900	-1.24738900	4.37213200
H	0.00000000	-2.48987100	4.38708600
H	-2.16221900	-1.24738900	4.37213200
H	-2.16221900	1.24738900	4.37213200
H	0.00000000	2.48987100	4.38708600
H	2.16221900	1.24738900	4.37213200

(5) C₆H₆MnB₄₀

B	-2.72780800	1.74288100	-1.67094400
B	0.00000000	1.75405300	1.63897800
B	-2.34913300	1.37303400	-0.08585400
B	2.72780800	-1.74288100	-1.67094400
B	1.68629900	0.00000000	-4.14967200
B	0.00000000	2.63045200	-3.25525400
B	0.88716100	-2.34152800	0.42003400
B	-1.39726300	-2.36411100	-2.48966500
B	-2.72780800	-1.74288100	-1.67094400
B	0.00000000	-1.75405300	1.63897800
B	-2.34913300	-1.37303400	-0.08585400
B	1.73153700	2.70448700	-0.89476900
B	2.34913300	1.37303400	-0.08585400
B	2.34913300	-1.37303400	-0.08585400
B	2.36914200	-0.87728700	-2.96631600
B	-2.36914200	0.87728700	-2.96631600
B	-0.88716100	-2.34152800	0.42003400
B	2.36914200	0.87728700	-2.96631600
B	2.64277900	0.00000000	0.70727600
B	-1.73153700	2.70448700	-0.89476900
B	-0.88716100	2.34152800	0.42003400
B	0.88716100	2.34152800	0.42003400
B	1.39726300	-2.36411100	-2.48966500
B	-1.39726300	2.36411100	-2.48966500
B	1.39726300	2.36411100	-2.48966500
B	1.40740000	-0.88662400	1.31207400
B	1.40740000	0.88662400	1.31207400
B	2.72780800	1.74288100	-1.67094400
B	0.88676200	1.38716200	-3.82053800
B	0.00000000	-2.63045200	-3.25525400
B	-2.36914200	-0.87728700	-2.96631600
B	-1.40740000	-0.88662400	1.31207400
B	-1.40740000	0.88662400	1.31207400
B	-0.88676200	1.38716200	-3.82053800
B	1.73153700	-2.70448700	-0.89476900
B	-2.64277900	0.00000000	0.70727600
B	0.88676200	-1.38716200	-3.82053800
B	-1.68629900	0.00000000	-4.14967200
B	-1.73153700	-2.70448700	-0.89476900
B	-0.88676200	-1.38716200	-3.82053800
C	1.23116800	-0.70026800	4.43314100
C	0.00000000	-1.39470600	4.40071600

C	-1.23116800	-0.70026800	4.43314100
C	-1.23116800	0.70026800	4.43314100
C	0.00000000	1.39470600	4.40071600
C	1.23116800	0.70026800	4.43314100
H	2.16499300	-1.25001100	4.39875600
H	0.00000000	-2.47786900	4.34334700
H	-2.16499300	-1.25001100	4.39875600
H	-2.16499300	1.25001100	4.39875600
H	0.00000000	2.47786900	4.34334700
H	2.16499300	1.25001100	4.39875600
Mn	0.00000000	0.00000000	2.76082300

(6) C₆H₆FeB₄₀

B	-2.71749400	1.73280700	-1.72324700
B	0.00000000	1.76713800	1.59313600
B	-2.34192400	1.38069200	-0.13107900
B	2.71749400	-1.73280700	-1.72324700
B	1.68190200	0.00000000	-4.21391300
B	0.00000000	2.63328100	-3.32198600
B	0.87432000	-2.35416700	0.35267900
B	-1.39600200	-2.36250800	-2.55474000
B	-2.71749400	-1.73280700	-1.72324700
B	0.00000000	-1.76713800	1.59313600
B	-2.34192400	-1.38069200	-0.13107900
B	1.72250800	2.70402800	-0.95956600
B	2.34192400	1.38069200	-0.13107900
B	2.34192400	-1.38069200	-0.13107900
B	2.36124700	-0.87466100	-3.02442700
B	-2.36124700	0.87466100	-3.02442700
B	-0.87432000	-2.35416700	0.35267900
B	2.36124700	0.87466100	-3.02442700
B	2.62907000	0.00000000	0.65514400
B	-1.72250800	2.70402800	-0.95956600
B	-0.87432000	2.35416700	0.35267900
B	0.87432000	2.35416700	0.35267900
B	1.39600200	-2.36250800	-2.55474000
B	-1.39600200	2.36250800	-2.55474000
B	1.39600200	2.36250800	-2.55474000
B	1.40211500	-0.90352200	1.25980800
B	1.40211500	0.90352200	1.25980800
B	2.71749400	1.73280700	-1.72324700
B	0.88653000	1.39092500	-3.88933000
B	0.00000000	-2.63328100	-3.32198600
B	-2.36124700	-0.87466100	-3.02442700

B	-1.40211500	-0.90352200	1.25980800
B	-1.40211500	0.90352200	1.25980800
B	-0.88653000	1.39092500	-3.88933000
B	1.72250800	-2.70402800	-0.95956600
B	-2.62907000	0.00000000	0.65514400
B	0.88653000	-1.39092500	-3.88933000
B	-1.68190200	0.00000000	-4.21391300
B	-1.72250800	-2.70402800	-0.95956600
B	-0.88653000	-1.39092500	-3.88933000
C	1.21537500	-0.70138400	4.64860600
C	0.00000000	-1.40086400	4.66368100
C	-1.21537500	-0.70138400	4.64860600
C	-1.21537500	0.70138400	4.64860600
C	0.00000000	1.40086400	4.66368100
C	1.21537500	0.70138400	4.64860600
H	2.15368800	-1.24406100	4.62470000
H	0.00000000	-2.48509300	4.64808300
H	-2.15368800	-1.24406100	4.62470000
H	-2.15368800	1.24406100	4.62470000
H	0.00000000	2.48509300	4.64808300
H	2.15368800	1.24406100	4.62470000
Fe	0.00000000	0.00000000	2.72879000

(7) C₆H₆CoB₄₀

B	3.66696900	1.23962900	1.96211900
B	1.30674400	-2.24359300	2.40483100
B	3.52837300	-0.42665000	2.02507300
B	-1.18555100	-0.47868300	-2.22878300
B	-0.64436900	2.51982600	-0.96516100
B	0.66209700	2.55699500	1.99573400
B	1.04420600	-2.27035400	-1.90482000
B	2.94607100	0.77281700	-2.37044200
B	4.24615000	0.34456900	-1.37089500
B	1.85739900	-3.09603600	-0.77666600
B	3.99500400	-1.14699200	-0.65431300
B	-0.83413800	0.12725600	2.56672400
B	-1.19458500	-1.07637400	1.42094900
B	-0.72668000	-1.82096100	-1.33214100
B	-1.05695500	1.04279400	-1.54731300
B	3.32342800	2.20380200	0.73316800
B	2.75345500	-2.04576800	-1.63263800
B	-1.35113700	1.49031300	0.10006200
B	-1.10713400	-2.22591700	0.22885400
B	2.61883800	0.62164300	2.98265900

B	1.97297600	-0.83796000	2.87256400
B	0.25258000	-1.04196900	2.65886700
B	0.15574400	0.36732800	-2.74373600
B	2.16017200	1.98975300	2.15892500
B	-0.62984600	1.58679100	1.78308600
B	0.32406600	-2.75951000	-0.32638900
B	0.02731200	-2.30127700	1.39103300
B	-1.80520700	0.48569900	1.35545200
B	-0.03184600	2.65987200	0.53724600
B	1.52541100	1.21691600	-2.98399900
B	3.61544200	1.75255200	-0.94776200
B	3.07567800	-2.41600400	0.07522700
B	2.78374400	-1.96365800	1.76200000
B	1.69769600	2.93172800	0.80422400
B	0.08271200	-1.30105100	-2.73575100
B	4.09301400	-1.46968400	0.92655400
B	0.41917500	1.95789800	-2.06329500
B	2.65581600	2.98808400	-0.51989000
B	3.52406700	-0.77802000	-2.23078700
B	2.16218700	2.21176900	-1.87176700
C	-4.44185200	0.45708500	-1.20211700
C	-4.38379500	-0.87569800	-0.77757400
C	-4.80838500	-1.20830800	0.51600100
C	-5.28852100	-0.22240300	1.36695900
C	-5.34686800	1.10279300	0.93869300
C	-4.91988700	1.44335700	-0.33768300
H	-4.16063400	0.71432100	-2.21802800
H	-4.11517700	-1.65927800	-1.48060200
H	-4.77334300	-2.24288300	0.84296000
H	-5.61911600	-0.48470900	2.36711500
H	-5.72490300	1.87103000	1.60622900
H	-4.96765100	2.47491700	-0.67206000
Co	-2.03884100	-0.43304500	-0.41353000

(8) C₆H₆NiB₄₀

B	3.65563500	0.99303000	2.10814800
B	1.32238000	-2.53619800	2.08962700
B	3.53050700	-0.66731000	1.95350000
B	-1.15062000	-0.18120200	-2.27885800
B	-0.65411900	2.62029400	-0.63687500
B	0.64968500	2.29623800	2.31088000
B	1.06517600	-2.00647400	-2.17765500
B	2.95048400	1.09590100	-2.24107000
B	4.24621500	0.54302700	-1.30279600

B	1.88429100	-2.96432800	-1.16607700
B	4.00507200	-1.02948800	-0.78565000
B	-0.82685500	-0.21165500	2.55351300
B	-1.16449100	-1.25632900	1.25296900
B	-0.68813500	-1.62966200	-1.54908700
B	-1.06554600	1.24571500	-1.42586800
B	3.30974100	2.10976900	1.01625200
B	2.76770900	-1.80305900	-1.87707000
B	-1.36983000	1.47638200	0.29272000
B	-1.09766900	-2.27117700	-0.06750100
B	2.60494300	0.24212300	3.03130300
B	1.97091300	-1.19596600	2.73510800
B	0.25792600	-1.38646200	2.49180900
B	0.18073100	0.73021400	-2.68387500
B	2.14853900	1.70787900	2.39459600
B	-0.62526800	1.34755500	1.97635700
B	0.34187800	-2.71344200	-0.67192000
B	0.04197900	-2.48665800	1.06771500
B	-1.78683200	0.30553100	1.39875900
B	-0.04228700	2.56857000	0.87078700
B	1.53428800	1.61858400	-2.80682500
B	3.60856800	1.88376200	-0.70525300
B	3.09894000	-2.39252900	-0.23262200
B	2.79969600	-2.16425200	1.49621800
B	1.68438500	2.82092300	1.17411300
B	0.11175100	-0.93254000	-2.88280300
B	4.11120200	-1.56260200	0.73789100
B	0.41860300	2.21499800	-1.79301800
B	2.64902300	3.05780800	-0.12455700
B	3.52738300	-0.46100700	-2.30029000
B	2.15808000	2.45815700	-1.56383100
C	-4.63686500	0.51209800	-1.18666100
C	-4.44878000	-0.82503700	-0.83004700
C	-4.75988300	-1.24714000	0.46497600
C	-5.24602800	-0.33676500	1.39602400
C	-5.42901700	0.99598100	1.03627200
C	-5.12538700	1.42068900	-0.25226100
H	-4.41615700	0.83748900	-2.19850000
H	-4.13212000	-1.54860700	-1.57596100
H	-4.62421400	-2.28883500	0.73952500
H	-5.48548500	-0.66589300	2.40253500
H	-5.81122300	1.70521600	1.76437500
H	-5.27046000	2.45962300	-0.53179600
Ni	-1.90017600	-0.39423400	-0.45585100