

Supporting information

Heptacoordinate Transition-Metal-Decorated Metallo-Borosphenes and Multiple-Helix Metallo-Boronanotubes

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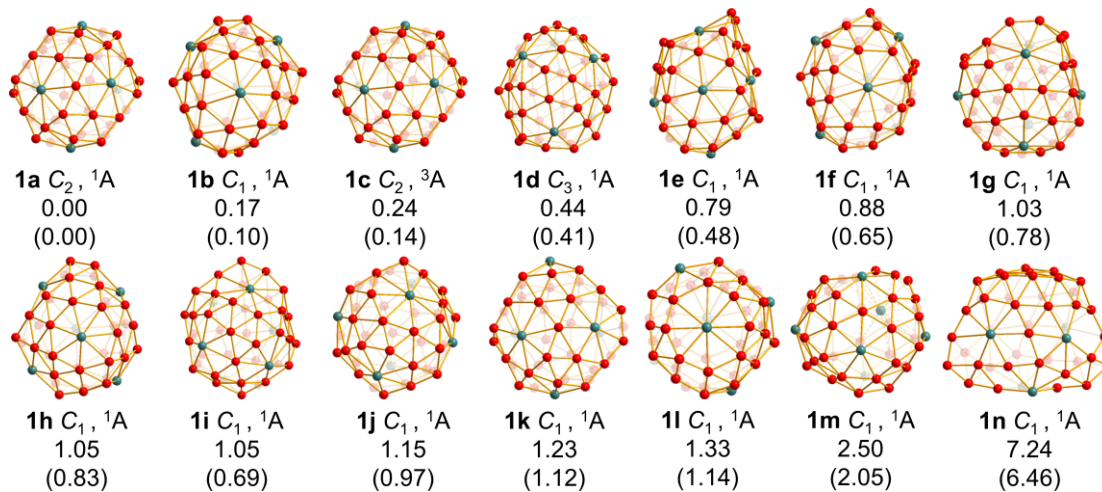
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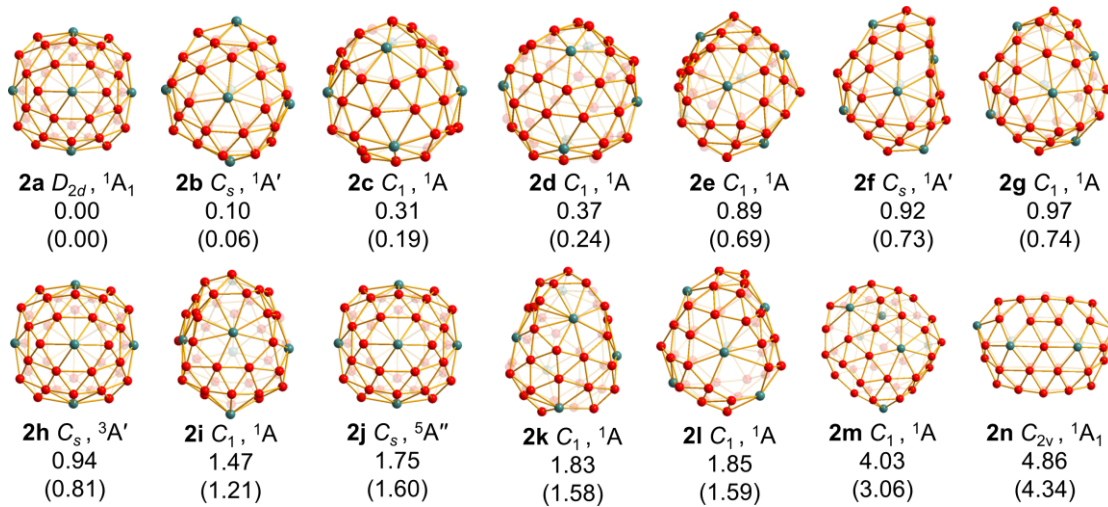
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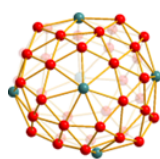
(a) $\text{Ni}_6\text{B}_{39}^-$



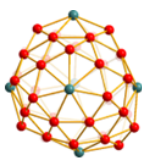
(b) Ni₆B₄₀



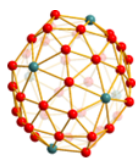
(c) $\text{Ni}_6\text{B}_{41}^+$



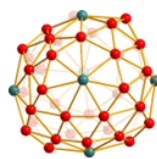
3a $C_1, ^1A$
0.00
(0.00)



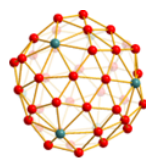
3b $C_1, ^1A$
0.08
(0.15)



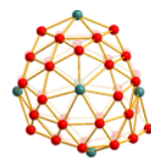
3c $C_2, ^1A$
0.19
(0.18)



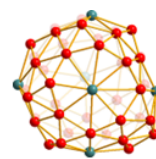
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0.25
(0.28)



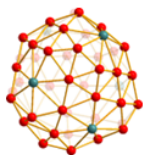
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(0.29)



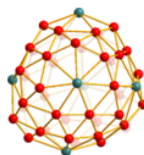
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(0.40)



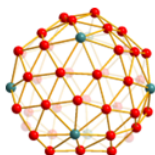
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(0.66)



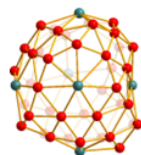
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(1.39)



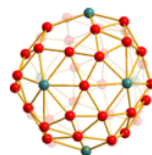
3i $C_1, ^1A$
1.54
(1.52)



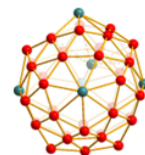
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(1.52)



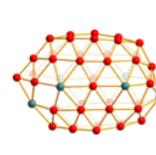
3k $C_1, ^1A$
1.84
(1.61)



3l $C_1, ^1A$
1.91
(1.87)

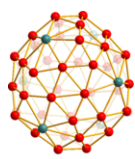


3m $C_1, ^1A$
2.52
(2.28)

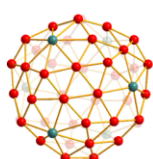


3n $C_1, ^1A$
5.78
(5.18)

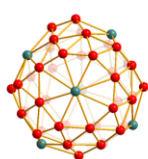
(d) $\text{Ni}_6\text{B}_{42}^{2+}$



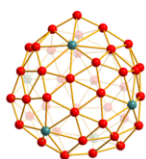
4a $C_2, ^1A$
0.00
(0.00)



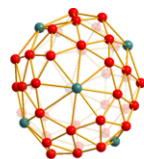
4b $D_3, ^1A_1$
0.28
(0.25)



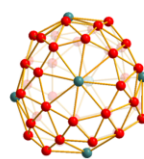
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0.61
(0.56)



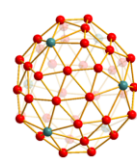
4d $C_1, ^1A$
0.65
(0.55)



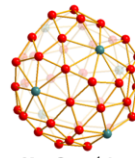
4e $C_1, ^1A$
0.69
(0.57)



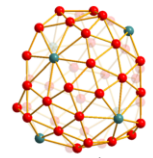
4f $C_1, ^1A$
0.97
(0.86)



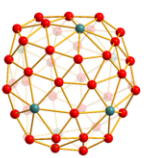
4g $C_1, ^3A$
1.02
(0.97)



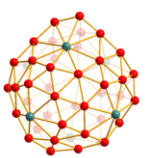
4h $C_1, ^1A$
1.08
(0.98)



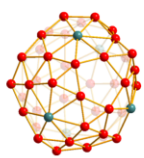
4i $C_1, ^1A$
1.19
(1.06)



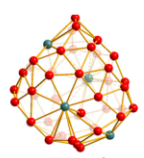
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1.21
(1.11)



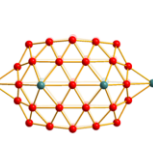
4k $C_1, ^1A$
1.23
(1.03)



4l $C_1, ^1A$
1.35
(1.20)

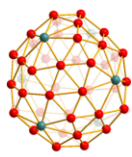


4m $C_1, ^1A$
4.29
(3.26)

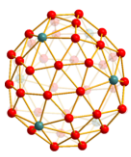


4n $D_{2h}, ^1A_1$
6.23
(6.01)

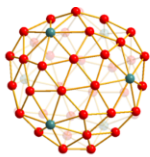
(e) Ni₆B₄₂



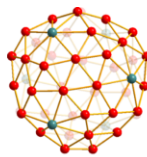
5a C_{2v}, ³B
0.00
(0.00)



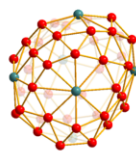
5b C₁, ¹A
0.05
(0.05)



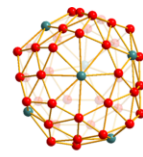
5c D_{3h}, ³A₁
0.05
(0.06)



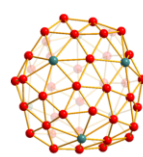
5d C₁, ¹A
0.07
(0.09)



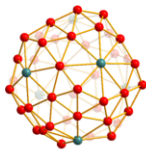
5e C₁, ¹A
0.18
(0.16)



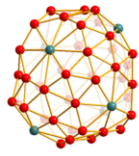
5f C₁, ¹A
0.59
(0.46)



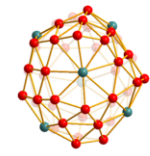
5g C₁, ³A
0.59
(0.58)



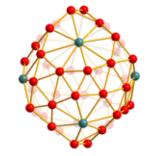
5h C₁, ³A
0.66
(0.64)



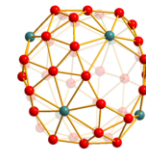
5i C₁, ¹A
0.69
(0.60)



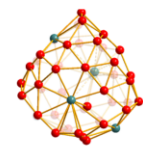
5j C₁, ³A
0.72
(0.59)



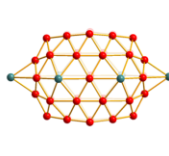
5k C₁, ¹A
0.90
(0.84)



5l C₁, ¹A
1.03
(0.92)

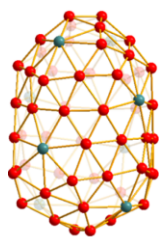


5m C₁, ¹A
3.30
(2.25)

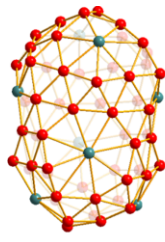


5n D_{2h}, ¹A₁
5.15
(5.26)

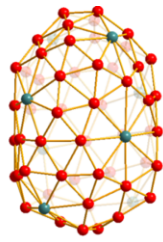
(f) Ni₈B₅₆



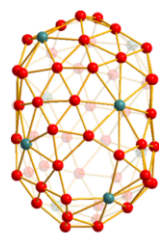
6a C₂, ¹A
0.00
(0.00)



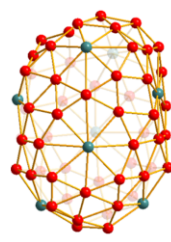
6b C₁, ¹A
0.29
(0.20)



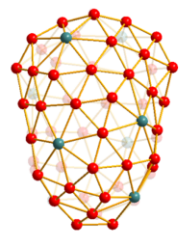
6c C₁, ¹A
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(0.29)



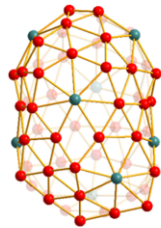
6d C₁, ¹A
1.12
(0.92)



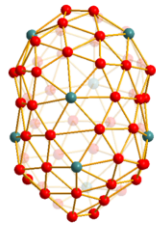
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1.17
(0.84)



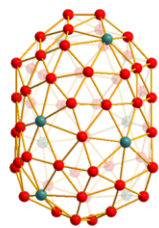
6f C₁, ¹A
1.25
(1.10)



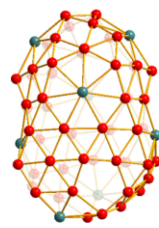
6g C₁, ¹A
1.33
(1.20)



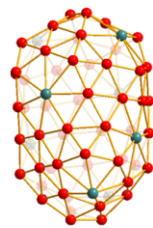
6h C₁, ¹A
1.63
(1.47)



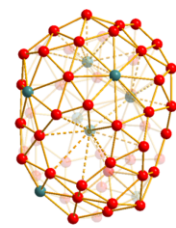
6i C₁, ¹A
1.64
(1.36)



6j C₁, ¹A
1.72
(1.62)



6k C₁, ¹A
1.80
(1.64)



6l C₁, ¹A
6.64
(6.48)

Figure S2. The optimized structures of $C_2 Ni_{10}B_{70}$, and $C_2 Ni_{12}B_{84}$.

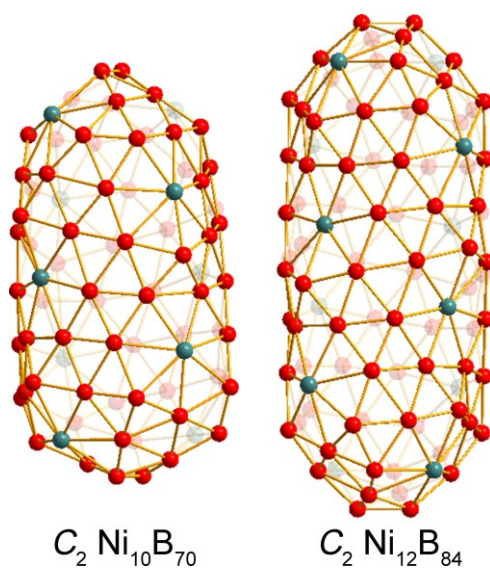


Figure S3. BOMD simulations of (a) C_2 $Ni_6 \in B_{39}^-$ (**1**), (b) D_{2d} $Ni_6 \in B_{40}$ (**2**), (c) C_1 $Ni_6 \in B_{41}^+$ (**3**), (d) C_2 $Ni_6 \in B_{42}^{2+}$ (**4**), (e) $Ni_6 \in B_{42}$ (**5**), and (f) $Ni_8 \in B_{56}$ (**6**) at different temperatures with the RMSD and MAXD indicated in Å.

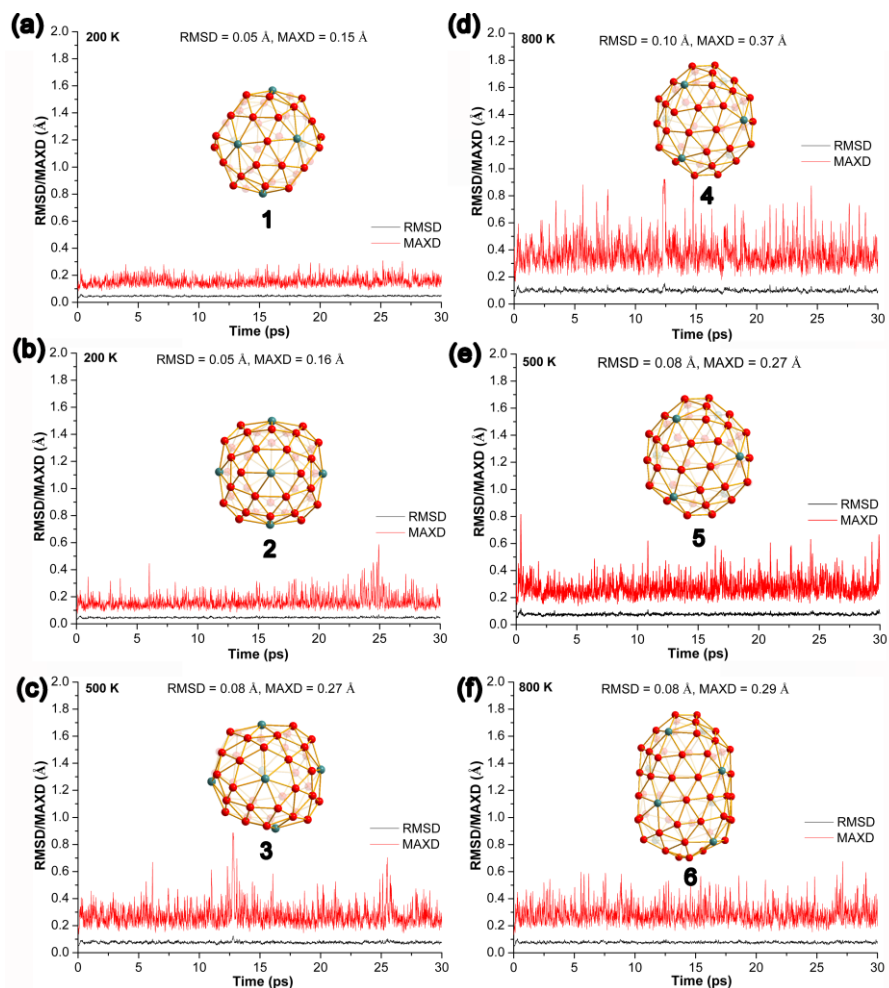


Figure S4. The optimized structures of 1D Ni/B binary nanotubes.

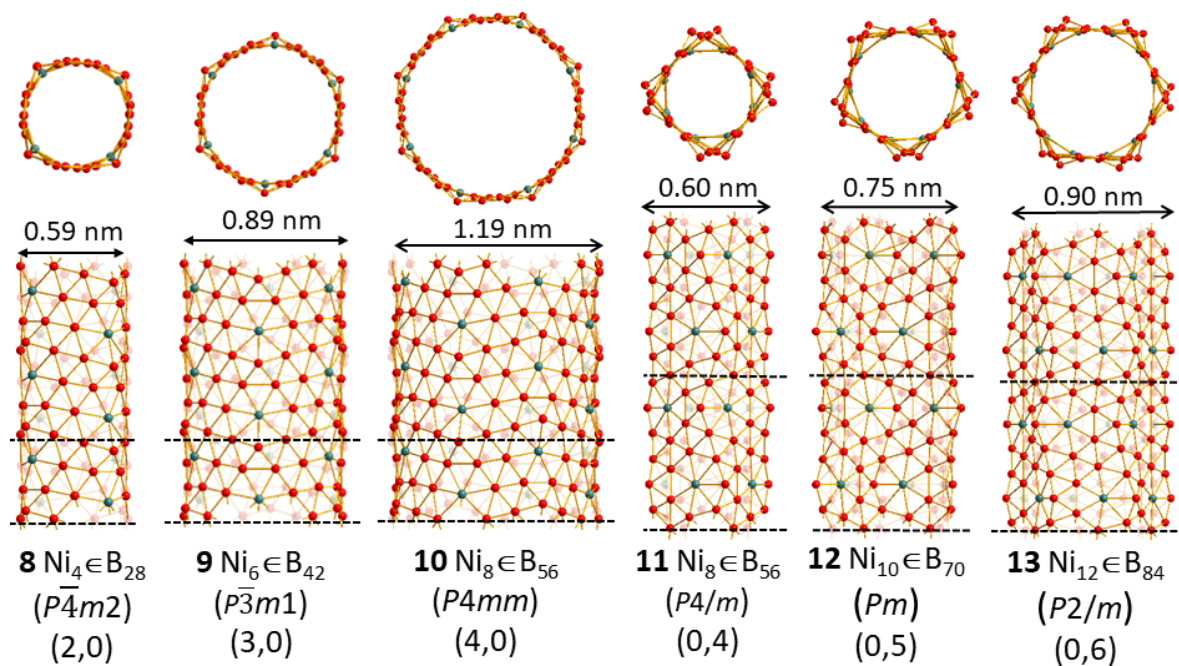


Figure S5. Band structure and PDOS of a series of 1D Ni/B binary nanotubes. (a)–(e) corresponds to nanotubes **8–13**.

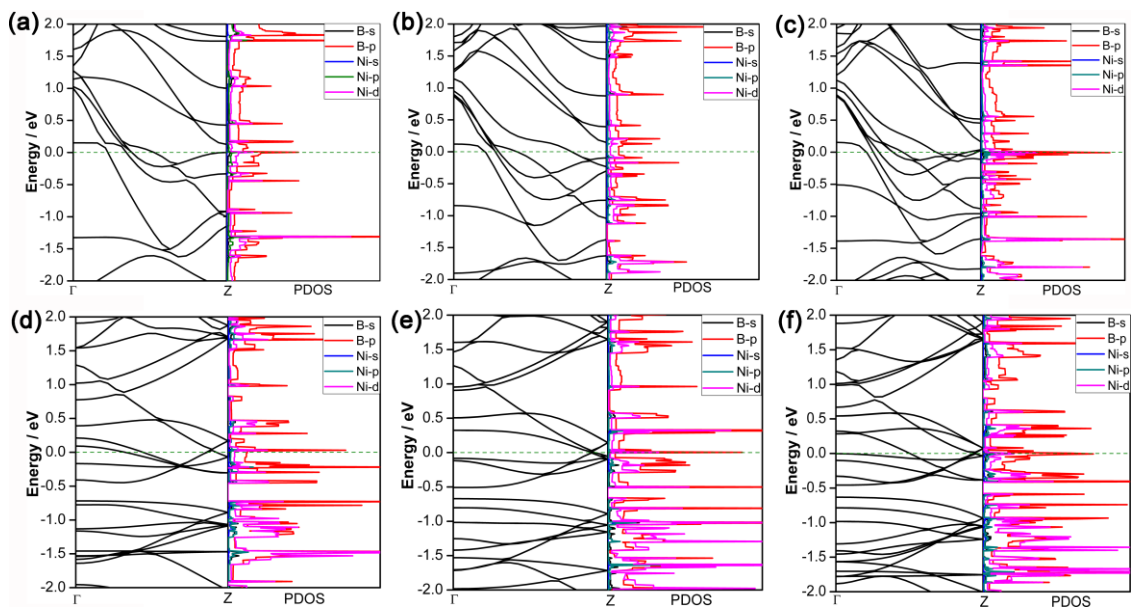


Table S1. Optimized cartesian coordinates (x, y, z) of (a) C_2 Ni₆&B₃₉⁻ (**1**), (b) D_{2d} Ni₆&B₄₀ (**2**), (c) C_1 Ni₆&B₄₁⁺ (**3**), (d) C_2 Ni₆&B₄₂²⁺ (**4**), (e) Ni₆B₄₂ (**5**), (f) Ni₈B₅₆ (**6**), (g) C_2 Ni₁₀&B₇₀ and (f) Ni₁₂&B₈₄ at PBE0/6-311+G(d) level.

(a) C_2 Ni₆&B₃₉⁻ (**1**)

B	-1.13770400	-3.03315600	-1.37782200
B	0.64585900	0.46011300	-3.34239500
B	0.46578800	-2.46223400	-1.50638900
B	-0.11132500	2.82142100	2.11784200
B	-2.45718600	1.45262700	1.22642000
B	-3.30920900	-0.62315700	-0.64469300
B	1.58916800	-2.80854300	1.37746500
B	3.30920900	0.62315700	-0.64469300
B	1.75277000	-2.40981900	-0.24489700
B	-1.95737900	1.84289500	-1.75277900
B	-0.46578800	2.46223400	-1.50638900
B	1.91260100	2.94068300	0.12624200
B	-1.03992800	1.44689400	2.30696500
B	-1.91260100	-2.94068300	0.12624200
B	-1.58916800	2.80854300	1.37746500
B	1.13770400	3.03315600	-1.37782200
B	-0.98011900	-1.81419300	-2.41118400
B	-0.64585900	-0.46011300	-3.34239500
B	-0.73680500	1.13663800	-2.65868700
B	-2.29165900	-1.84300500	-1.11682500
B	-2.75817100	0.97065100	-0.55670400
B	2.29165900	1.84300500	-1.11682500
B	0.98011900	1.81419300	-2.41118400
B	-1.75277000	2.40981900	-0.24489700
B	-3.26816300	0.08799700	0.77836100
B	0.11132500	-2.82142100	2.11784200
B	2.75817100	-0.97065100	-0.55670400
B	0.73680500	-1.13663800	-2.65868700
B	-2.66476100	-1.54766100	0.64827600
B	1.95737900	-1.84289500	-1.75277900
B	0.00000000	0.00000000	2.94904700
B	-1.47721200	-2.33056000	1.62301600
B	-0.55180900	-1.55711600	2.86832400
B	2.66476100	1.54766100	0.64827600
B	3.26816300	-0.08799700	0.77836100
B	2.45718600	-1.45262700	1.22642000
B	1.47721200	2.33056000	1.62301600
B	1.03992800	-1.44689400	2.30696500
B	0.55180900	1.55711600	2.86832400
Ni	0.00000000	3.37478400	0.25086000
Ni	1.89273700	0.33879900	2.14136900
Ni	-1.89273700	-0.33879900	2.14136900
Ni	-2.24062400	-0.12742700	-2.20206100
Ni	2.24062400	0.12742700	-2.20206100
Ni	0.00000000	-3.37478400	0.25086000

(b) D_{2d} Ni₆&B₄₀ (2)

B	2.84397900	1.88207700	0.40731600
B	0.00000000	1.81351100	-2.90783400
B	2.42609600	1.47623400	-1.23193800
B	-2.84397900	-1.88207700	0.40731600
B	-1.81351100	0.00000000	2.90783400
B	0.00000000	2.64116900	1.99950400
B	-0.89993800	-2.43010900	-1.68005900
B	1.47623400	-2.42609600	1.23193800
B	2.84397900	-1.88207700	0.40731600
B	0.00000000	-1.81351100	-2.90783400
B	2.42609600	-1.47623400	-1.23193800
B	-1.88207700	2.84397900	-0.40731600
B	-2.42609600	1.47623400	-1.23193800
B	-2.42609600	-1.47623400	-1.23193800
B	-2.43010900	-0.89993800	1.68005900
B	2.43010900	0.89993800	1.68005900
B	0.89993800	-2.43010900	-1.68005900
B	-2.43010900	0.89993800	1.68005900
B	-2.64116900	0.00000000	-1.99950400
B	1.88207700	2.84397900	-0.40731600
B	0.89993800	2.43010900	-1.68005900
B	-0.89993800	2.43010900	-1.68005900
B	-1.47623400	-2.42609600	1.23193800
B	1.47623400	2.42609600	1.23193800
B	-1.47623400	2.42609600	1.23193800
B	-1.42643600	-0.93815100	-2.56370900
B	-1.42643600	0.93815100	-2.56370900
B	-2.84397900	1.88207700	0.40731600
B	-0.93815100	1.42643600	2.56370900
B	0.00000000	-2.64116900	1.99950400
B	2.43010900	-0.89993800	1.68005900
B	1.42643600	-0.93815100	-2.56370900
B	1.42643600	0.93815100	-2.56370900
B	0.93815100	1.42643600	2.56370900
B	-1.88207700	-2.84397900	-0.40731600
B	2.64116900	0.00000000	-1.99950400
B	-0.93815100	-1.42643600	2.56370900
B	1.81351100	0.00000000	2.90783400
B	1.88207700	-2.84397900	-0.40731600
B	0.93815100	-1.42643600	2.56370900
Ni	0.00000000	3.14132000	0.03882000
Ni	0.00000000	-3.14132000	0.03882000
Ni	3.14132000	0.00000000	-0.03882000
Ni	-3.14132000	0.00000000	-0.03882000
Ni	0.00000000	0.00000000	3.61982400
Ni	0.00000000	0.00000000	-3.61982400

(c) $C_1 Ni_6 \& B_{41}^+$ (3)

B	1.27854600	3.31275100	0.22728000
B	-1.55186700	2.95335700	-0.27949900
B	0.38601300	0.83327800	2.89734100
B	-1.80634000	2.14449200	1.44118600
B	-1.97739400	0.76933400	-2.25475100
B	0.13460400	-1.24343700	-2.57210400
B	1.19086000	2.60957100	-1.31601100
B	1.41564100	-0.02106200	-2.58076000
B	-0.25220900	-3.48981200	-0.53242400
B	-1.17749100	-2.15592600	1.88794900
B	1.14559100	-2.97924500	0.24802400
B	-2.63734900	-0.79471800	-1.60272000
B	-2.63171300	-1.54024200	1.02148200
B	1.18982100	-0.60974500	3.16549400
B	2.78369600	0.82237100	1.22963400
B	3.02331200	-0.71919600	0.29442600
B	-0.32418500	-3.33597400	1.05577500
B	2.10059900	0.60173300	2.72116800
B	-0.42585800	-0.81156700	2.83076500
B	-1.33674800	0.72306100	2.45746500
B	0.68758400	-2.64296300	-1.58943500
B	2.35284300	-0.85083600	1.91151800
B	2.20354100	-2.01566400	-0.76883900
B	-0.25112000	3.01832500	1.00794500
B	-1.67345400	-2.87684000	0.22260000
B	-1.44859500	-0.66874900	-2.77785000
B	-2.52893100	2.07912700	-1.37826200
B	-3.60983600	-0.76568300	-0.21801000
B	2.38115900	2.11120000	0.04512100
B	-0.25808000	0.49146700	-2.75873800
B	2.30353500	1.30364900	-1.59435100
B	-0.05786300	3.56639200	-0.56542900
B	3.34242900	0.83751800	-0.32018400
B	-0.53150400	2.16734800	2.43443100
B	1.73123600	-1.68434700	-2.36998400
B	-2.93438800	-2.14733200	-0.52317700
B	-2.88808200	2.10218500	0.18605900
B	1.04269900	1.56811200	-2.60160800
B	-2.00161200	-0.84604400	2.40586600
B	2.45107100	-2.13977800	0.84557500
B	-3.21868600	0.71752000	-0.76098900
Ni	3.14824400	-0.51609600	-1.70426800
Ni	0.87796300	-2.24295200	2.13136400
Ni	-2.97393700	0.45859400	1.27437000
Ni	1.41360800	2.23636300	1.87181000
Ni	-0.69552100	2.34922700	-2.04454500
Ni	-1.34562000	-2.35542700	-1.73801300

(d) C₂ Ni₆&B₄₂²⁺ (4)

B	1.27352100	0.61873300	-3.10908100
B	-1.27352100	-0.61873300	-3.10908100
B	-1.39095200	2.30724600	-1.11555600
B	-2.61322100	-0.21449100	-1.91927200
B	-0.01615200	-3.13463800	-0.64433900
B	2.04396300	-2.29674800	1.72628400
B	1.59645700	-1.19223300	-2.52055300
B	2.52933200	-1.86673700	0.19005300
B	0.46542500	-0.63232300	3.62586900
B	-2.04396300	2.29674800	1.72628400
B	1.14450300	0.75929100	2.97315000
B	-0.84284900	-2.67569400	0.71058700
B	-2.53944800	-0.55549200	1.83541500
B	-0.95534100	2.81455700	0.60140100
B	1.54066100	2.51627500	-0.91386900
B	2.44622500	1.79135900	0.53151600
B	-1.79363300	0.93902400	2.73142100
B	0.01615200	3.13463800	-0.64433900
B	-2.52933200	1.86673700	0.19005300
B	-2.73457200	1.38340300	-1.39698400
B	1.79363300	-0.93902400	2.73142100
B	0.84284900	2.67569400	0.71058700
B	2.53944800	0.55549200	1.83541500
B	-0.37889800	0.70685900	-3.53531800
B	-1.14450300	-0.75929100	2.97315000
B	0.95534100	-2.81455700	0.60140100
B	-1.54066100	-2.51627500	-0.91386900
B	-2.44622500	-1.79135900	0.53151600
B	2.16197900	1.76938100	-2.35889500
B	1.39095200	-2.30724600	-1.11555600
B	2.61322100	0.21449100	-1.91927200
B	0.37889800	-0.70685900	-3.53531800
B	2.97714300	1.65085400	-1.02119100
B	-1.59645700	1.19223300	-2.52055300
B	3.00758100	-1.03559000	1.62106100
B	-1.73683200	-1.97277400	1.98558400
B	-2.16197900	-1.76938100	-2.35889500
B	2.73457200	-1.38340300	-1.39698400
B	-3.00758100	1.03559000	1.62106100
B	1.73683200	1.97277400	1.98558400
B	-2.97714300	-1.65085400	-1.02119100
B	-0.46542500	0.63232300	3.62586900
Ni	0.18512600	-2.22361400	2.41092900
Ni	-0.18512600	2.22361400	2.41092900
Ni	-0.18512600	-2.22005300	-2.39934400
Ni	0.18512600	2.22005300	-2.39934400
Ni	-3.31443100	0.00273700	-0.01110000
Ni	3.31443100	-0.00273700	-0.01110000

(e) $C_2 Ni_6 B_{42}$ (5)

B	1.30601000	0.58075300	-3.11357400
B	-1.30601000	-0.58075300	-3.11357400
B	-1.36422300	2.29241500	-1.12200200
B	-2.60620900	-0.19843400	-1.90754700
B	-0.03644300	-3.12983800	-0.64057700
B	2.02871400	-2.33537500	1.71913500
B	1.56460800	-1.15567700	-2.51109800
B	2.50589200	-1.86785700	0.18454600
B	0.47233400	-0.62519700	3.67957200
B	-2.02871400	2.33537500	1.71913500
B	1.14941000	0.74078500	2.94318800
B	-0.87133300	-2.63359800	0.70915400
B	-2.53412900	-0.52353400	1.83421900
B	-0.94379700	2.85513700	0.60749600
B	1.56460800	2.47340300	-0.90371500
B	2.44308300	1.76913200	0.50630000
B	-1.76686800	0.94760100	2.72912300
B	0.03644300	3.12983800	-0.64057700
B	-2.50589200	1.86785700	0.18454600
B	-2.73073000	1.40951900	-1.39848200
B	1.76686800	-0.94760100	2.72912300
B	0.87133300	2.63359800	0.70915400
B	2.53412900	0.52353400	1.83421900
B	-0.38526700	0.70457700	-3.58474800
B	-1.14941000	-0.74078500	2.94318800
B	0.94379700	-2.85513700	0.60749600
B	-1.56460800	-2.47340300	-0.90371500
B	-2.44308300	-1.76913200	0.50630000
B	2.19668000	1.74523300	-2.38679300
B	1.36422300	-2.29241500	-1.12200200
B	2.60620900	0.19843400	-1.90754700
B	0.38526700	-0.70457700	-3.58474800
B	3.02273900	1.64376300	-1.03176700
B	-1.56460800	1.15567700	-2.51109800
B	2.99724700	-1.07037000	1.62391800
B	-1.77144300	-1.96050800	1.99305100
B	-2.19668000	-1.74523300	-2.38679300
B	2.73073000	-1.40951900	-1.39848200
B	-2.99724700	1.07037000	1.62391800
B	1.77144300	1.96050800	1.99305100
B	-3.02273900	-1.64376300	-1.03176700
B	-0.47233400	0.62519700	3.67957200
Ni	0.16206400	-2.18030600	2.39374100
Ni	-0.16206400	2.18030600	2.39374100
Ni	-0.21203100	-2.17571700	-2.37353300
Ni	0.21203100	2.17571700	-2.37353300
Ni	-3.29191200	0.02819700	-0.00760100
Ni	3.29191200	-0.02819700	-0.00760100

(f) of $C_2 Ni_8 B_{56}$ (6)

B	0.79403200	-1.17324000	-4.29637200
B	-0.79403200	1.17324000	-4.29637200
B	2.11521600	1.60948900	-2.29015700
B	-0.53256900	2.50689500	-3.06890700
B	-3.17116300	-0.36264600	-1.92273700
B	-0.99136800	-1.73149900	-3.68117300
B	-1.57716600	-2.63868000	-0.84185200
B	-1.21996800	2.53606100	0.64105200
B	2.69215700	-1.22449100	-2.13124500
B	2.32785700	-2.25069300	-0.67312800
B	3.17116300	0.36264600	-1.92273700
B	1.57716600	2.63868000	-0.84185200
B	0.99635800	2.82666600	-2.48784300
B	1.21996800	-2.53606100	0.64105200
B	0.64791400	0.46636500	-4.72970700
B	-2.69215700	1.22449100	-2.13124500
B	-2.32785700	2.25069300	-0.67312800
B	2.03166600	-1.94627000	-3.57772400
B	-2.11521600	-1.60948900	-2.29015700
B	0.53256900	-2.50689500	-3.06890700
B	-0.64791400	-0.46636500	-4.72970700
B	2.07119000	-2.78853800	-2.23479500
B	0.99136800	1.73149900	-3.68117300
B	-0.55477700	-2.80924900	0.58205100
B	-2.03166600	1.94627000	-3.57772400
B	-0.99635800	-2.82666600	-2.48784300
B	0.55477700	2.80924900	0.58205100
B	-2.07119000	2.78853800	-2.23479500
B	-1.21996800	-2.75141200	2.17434200
B	-2.52083600	-0.54064500	3.07994400
B	-0.36412800	3.12520400	1.90274200
B	2.26148100	2.32615300	0.63072600
B	-2.89650500	0.55534000	-0.58032900
B	1.63436400	-2.07058400	2.25634300
B	2.65881000	-1.54701400	0.87409200
B	0.36412800	-3.12520400	1.90274200
B	-2.26148100	-2.32615300	0.63072600
B	-2.74905400	-2.03826700	2.22776100
B	2.89650500	-0.55534000	-0.58032900
B	-1.63436400	2.07058400	2.25634300
B	-2.65881000	1.54701400	0.87409200
B	1.21996800	2.75141200	2.17434200
B	2.52083600	0.54064500	3.07994400
B	2.87074300	-1.00533600	2.50065300
B	2.57875800	1.22133900	-0.65752000
B	2.74905400	2.03826700	2.22776100
B	-2.57875800	-1.22133900	-0.65752000
B	-2.87074300	1.00533600	2.50065300
B	0.47787400	-0.65302700	4.76504300
B	1.18116400	0.74685900	4.27938200
B	-1.70628400	0.93025700	3.66415700

B	1.70628400	-0.93025700	3.66415700
B	-1.18116400	-0.74685900	4.27938200
B	-1.93029300	-2.03979500	3.57322200
B	1.93029300	2.03979500	3.57322200
B	-0.47787400	0.65302700	4.76504300
Ni	-2.22294600	-0.08237200	-3.61908600
Ni	2.22294600	0.08237200	-3.61908600
Ni	0.09790300	-2.20191800	3.62282300
Ni	-0.09790300	2.20191800	3.62282300
Ni	3.01907400	0.43615300	1.10691000
Ni	-3.01907400	-0.43615300	1.10691000
Ni	-0.42702800	3.00023400	-1.10672400
Ni	0.42702800	-3.00023400	-1.10672400

(g) C₂ Ni₁₀&B₇₀

B	-1.82737700	2.33099300	-0.45728300
B	-1.00474500	-2.75189600	-1.72957200
B	1.00474500	2.75189600	-1.72957200
B	1.82737700	-2.33099300	-0.45728300
B	-2.83304000	0.99804200	-0.66556400
B	2.57219400	1.97205500	-1.88326700
B	-2.57219400	-1.97205500	-1.88326700
B	2.83304000	-0.99804200	-0.66556400
B	-2.87031800	-0.89122300	-0.60053600
B	2.27983200	-1.84963300	-2.01350800
B	-2.27983200	1.84963300	-2.01350800
B	2.87031800	0.89122300	-0.60053600
B	0.78421700	-2.64749800	-1.77544000
B	2.00332400	2.34347800	-0.31318000
B	-0.78421700	2.64749800	-1.77544000
B	-2.00332400	-2.34347800	-0.31318000
B	-3.51384600	0.09292000	0.47602400
B	3.51384600	-0.09292000	0.47602400
B	0.05224600	3.40506800	1.85390500
B	-0.05224600	-3.40506800	1.85390500
B	-2.73403700	1.60327000	0.94028700
B	2.73403700	-1.60327000	0.94028700
B	1.50251400	2.55751900	1.40588500
B	-1.50251400	-2.55751900	1.40588500
B	1.45092700	-2.66200700	1.33219900
B	-1.45092700	2.66200700	1.33219900
B	2.71461400	1.38725200	1.02889400
B	-2.71461400	-1.38725200	1.02889400
B	1.27940600	0.61287100	-5.48049300
B	-1.27940600	-0.61287100	-5.48049300
B	-1.25755700	2.28481800	-3.41509900
B	-2.55513000	-0.16632200	-4.23546300
B	-0.12367500	-3.17906500	-3.05501900
B	1.96793700	-2.40906400	4.13150800
B	1.55769100	-1.23034100	-4.84731400
B	2.46572000	-2.02322300	2.53689400
B	0.44383600	-0.64752100	6.01256200
B	-1.96793700	2.40906400	4.13150800
B	1.13568400	0.71101400	5.26011300
B	-0.89422500	-2.70383600	3.06382300
B	-2.46572000	-0.45462200	4.10858100
B	-0.91816900	3.05060000	3.04864700
B	1.61521700	2.48625600	-3.29989700
B	2.15913600	1.55378800	2.64927400
B	-1.73950900	1.03112500	5.08548500
B	0.12367500	3.17906500	-3.05501900
B	-2.46572000	2.02322300	2.53689400
B	-2.64051800	1.38924200	-3.66318200
B	1.73950900	-1.03112500	5.08548500
B	0.89422500	2.70383600	3.06382300
B	2.46572000	0.45462200	4.10858100

B	-0.36971200	0.71146900	-5.90354100
B	-1.13568400	-0.71101400	5.26011300
B	0.91816900	-3.05060000	3.04864700
B	-1.61521700	-2.48625600	-3.29989700
B	-2.15913600	-1.55378800	2.64927400
B	2.23631600	1.72922800	-4.77734900
B	1.25755700	-2.28481800	-3.41509900
B	2.55513000	0.16632200	-4.23546300
B	0.36971200	-0.71146900	-5.90354100
B	3.07627600	1.64562800	-3.44658100
B	-1.55769100	1.23034100	-4.84731400
B	2.92238100	-1.15515500	3.95371400
B	-1.74510200	-1.88468300	4.25107300
B	-2.23631600	-1.72922800	-4.77734900
B	2.64051800	-1.38924200	-3.66318200
B	-2.92238100	1.15515500	3.95371400
B	1.74510200	1.88468300	4.25107300
B	-3.07627600	-1.64562800	-3.44658100
B	-0.44383600	0.64752100	6.01256200
Ni	0.11814300	-2.25243500	4.79622400
Ni	-0.11814300	2.25243500	4.79622400
Ni	-3.22174100	0.11595500	2.35364400
Ni	3.22174100	-0.11595500	2.35364400
Ni	0.06322600	2.78692100	0.01577400
Ni	-0.06322600	-2.78692100	0.01577400
Ni	-3.22554100	0.01212200	-2.32696800
Ni	3.22554100	-0.01212200	-2.32696800
Ni	0.24683400	2.19696000	-4.76306300
Ni	-0.24683400	-2.19696000	-4.76306300

(f) C₂ Ni₁₂&B₈₄

B	-2.91111200	1.52676800	0.26140900
B	1.23275200	2.91194100	-2.60711800
B	-1.17925500	2.91467300	2.56175900
B	2.76390200	1.58112800	-0.23838900
B	-2.60122400	1.80149500	-1.43367200
B	0.40270400	3.06800800	3.34150600
B	-0.37684000	3.07712200	-3.26815000
B	2.65002700	1.77257400	1.42111600
B	-1.39168700	1.77080400	-2.78830300
B	2.85932100	3.14469900	0.43610900
B	-2.86539800	3.18835700	-0.43467400
B	1.40833100	1.74599600	2.79777700
B	2.37553500	2.92385600	-1.20045500
B	-0.25835800	1.53759900	3.15379900
B	-2.33886500	2.92415500	1.19189700
B	0.29413800	1.52165700	-3.15851400
B	-2.44649800	0.60714200	-2.49860100
B	2.42481800	0.54919600	2.45634600
B	-2.42481800	-0.54919600	2.45634600
B	2.44649800	-0.60714200	-2.49860100
B	-2.80779400	0.21102700	-0.84113700
B	2.93410300	0.13867200	0.84866300
B	-0.88215300	-0.16439800	3.05337100
B	0.85208700	-0.15686100	-3.04429200
B	2.80779400	-0.21102700	-0.84113700
B	-2.93410300	-0.13867200	0.84866300
B	0.88215300	0.16439800	3.05337100
B	-0.85208700	0.15686100	-3.04429200
B	0.44900200	6.68281100	1.36585900
B	-0.46367500	6.62602300	-1.31447100
B	-2.47123200	4.54024100	0.62671600
B	-1.65106200	5.45184500	-1.97099500
B	2.16071600	4.20701600	-2.22362700
B	1.92646500	5.99645700	0.30334200
B	2.91111200	-1.52676800	0.26140900
B	-1.23275200	-2.91194100	-2.60711800
B	-0.67790600	4.50118000	2.91417500
B	0.25835800	-1.53759900	3.15379900
B	-2.15279900	4.19203600	2.24439100
B	-2.76390200	-1.58112800	-0.23838900
B	-2.84506300	4.84240400	-0.96910400
B	1.17925500	-2.91467300	2.56175900
B	-0.77386900	7.08552700	0.24891000
B	0.66666000	4.49713400	-2.89753900
B	-0.29413800	-1.52165700	-3.15851400
B	0.29205200	5.96812300	2.82331400
B	2.51283200	4.57382600	-0.62971200
B	1.64560300	5.41338300	1.99014700
B	0.77133300	7.09569800	-0.19216100
B	0.93986800	4.65389900	3.39348000
B	-1.95286200	6.03355100	-0.30202600

B	2.33886500	-2.92415500	1.19189700
B	-0.29205200	5.98161300	-2.81221800
B	2.81059100	4.81541400	0.97847800
B	-2.37553500	-2.92385600	-1.20045500
B	-0.94960100	4.66461600	-3.37190500
Ni	-1.93822200	-1.18552500	-2.00392800
Ni	1.80795200	-1.18660900	1.90304100
Ni	-1.80795200	1.18660900	1.90304100
Ni	1.93822200	1.18552500	-2.00392800
Ni	-2.17912900	3.51566300	-2.31763800
Ni	2.23350600	3.49340500	2.36277000
Ni	-1.43709200	5.94311600	1.69244600
Ni	1.41048800	5.94614400	-1.67517200
B	0.46367500	-6.62602300	-1.31447100
B	-0.44900200	-6.68281100	1.36585900
B	-2.51283200	-4.57382600	-0.62971200
B	-1.64560300	-5.41338300	1.99014700
B	2.15279900	-4.19203600	2.24439100
B	1.95286200	-6.03355100	-0.30202600
B	2.86539800	-3.18835700	-0.43467400
B	-1.40833100	-1.74599600	2.79777700
B	-0.66666000	-4.49713400	-2.89753900
B	0.37684000	-3.07712200	-3.26815000
B	-2.16071600	-4.20701600	-2.22362700
B	-2.85932100	-3.14469900	0.43610900
B	-2.81059100	-4.81541400	0.97847800
B	1.39168700	-1.77080400	-2.78830300
B	-0.77133300	-7.09569800	-0.19216100
B	0.67790600	-4.50118000	2.91417500
B	-0.40270400	-3.06800800	3.34150600
B	0.29205200	-5.98161300	-2.81221800
B	2.47123200	-4.54024100	0.62671600
B	1.65106200	-5.45184500	-1.97099500
B	0.77386900	-7.08552700	0.24891000
B	0.94960100	-4.66461600	-3.37190500
B	-1.92646500	-5.99645700	0.30334200
B	2.60122400	-1.80149500	-1.43367200
B	-0.29205200	-5.96812300	2.82331400
B	2.84506300	-4.84240400	-0.96910400
B	-2.65002700	-1.77257400	1.42111600
B	-0.93986800	-4.65389900	3.39348000
Ni	1.43709200	-5.94311600	1.69244600
Ni	-1.41048800	-5.94614400	-1.67517200
Ni	-2.23350600	-3.49340500	2.36277000
Ni	2.17912900	-3.51566300	-2.31763800