Supporting Information

Lewis acid sites and flexible active center synergistically boost efficient electrochemical ammonia synthesis

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Supplementary Figs.
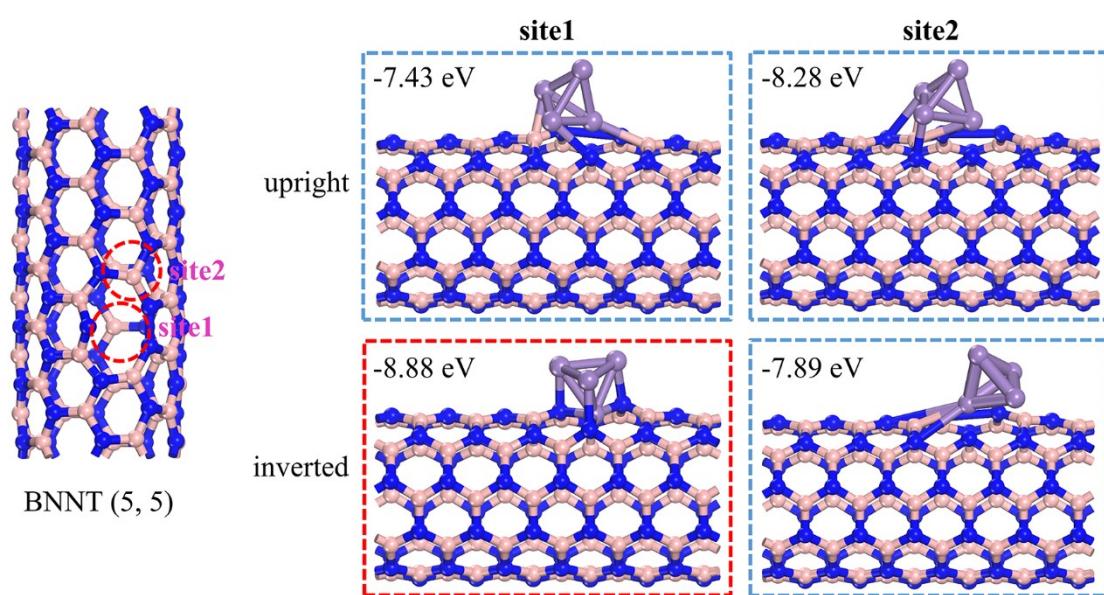
**Fig. S1** Binding energy for Mn_4 cluster coupling with (5, 5) BNNT through different sites and forms of orientation.
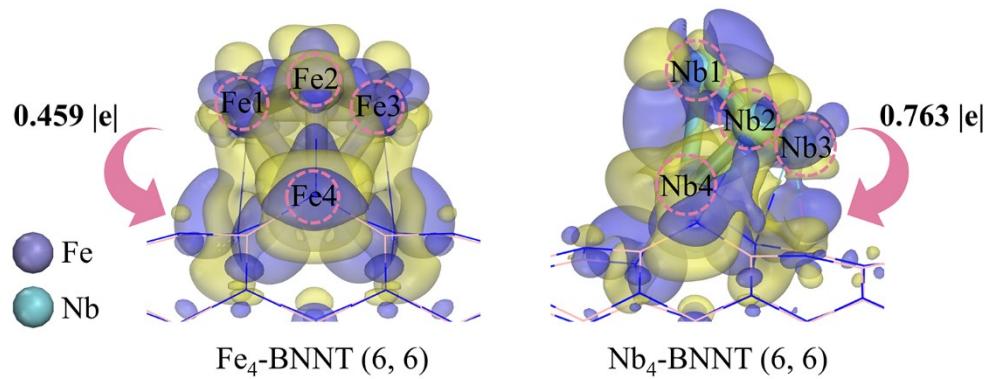
Fig. S2 Electron density difference and corresponding charge transfer (from TM_4 to BNNT substrate) for Fe_4/BNNT (6, 6) and Nb_4/BNNT (6, 6). Isosurface value is 0.0008 $e/Å^3$, where the blue and yellow isosurface indicate electron density accumulation and depletion, respectively.
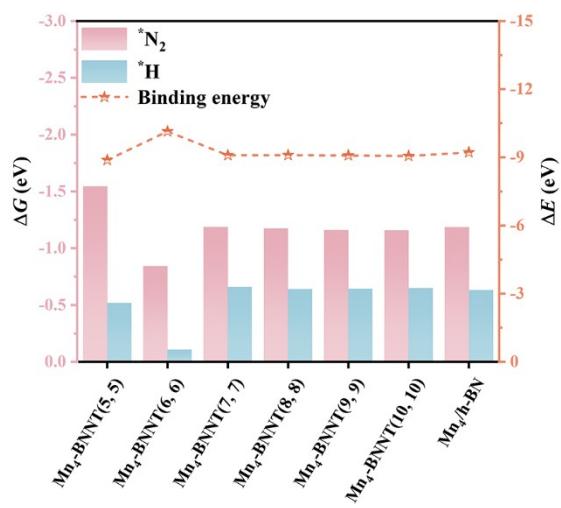
Fig. S3 Binding energy of Mn$_4$/BNNT (n, n) (n = 5, 6, 7, 8, 9, 10) with different armchair chirality, along with Mn$_4$/h-BN monolayer. ΔG for chemisorption of *N$_2$ and *H is also depicted in the figure.
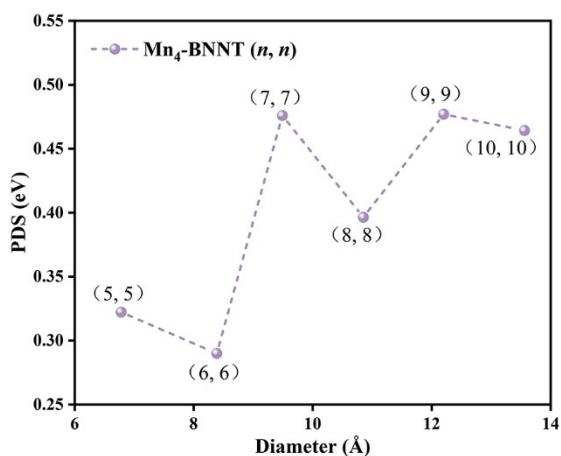
Fig. S4 A schematic diagram illustrating the reaction free energy for the PDS of Mn$_4$/BNNT (n, n) as a function of diameter.

Mn$_4$/BNNT(5, 5)
ΔG_{*N_2} = -1.54 eV

1.292 Å

D = 6.780 Å

Mn$_4$/BNNT(7, 7)
ΔG_{*N_2} = -1.19 eV

1.289 Å

D = 9.490 Å

Mn$_4$/BNNT(8, 8)
ΔG_{*N_2} = -1.17 eV

1.288 Å

D = 10.850 Å

Mn$_4$/BNNT(9, 9)
ΔG_{*N_2} = -1.16 eV

1.290 Å

D = 12.200 Å

Mn$_4$/BNNT(10, 10)
ΔG_{*N_2} = -1.16 eV

1.289 Å

D = 13.560 Å

Mn$_4$/h-BN
ΔG_{*N_2} = -1.19 eV

1.290 Å
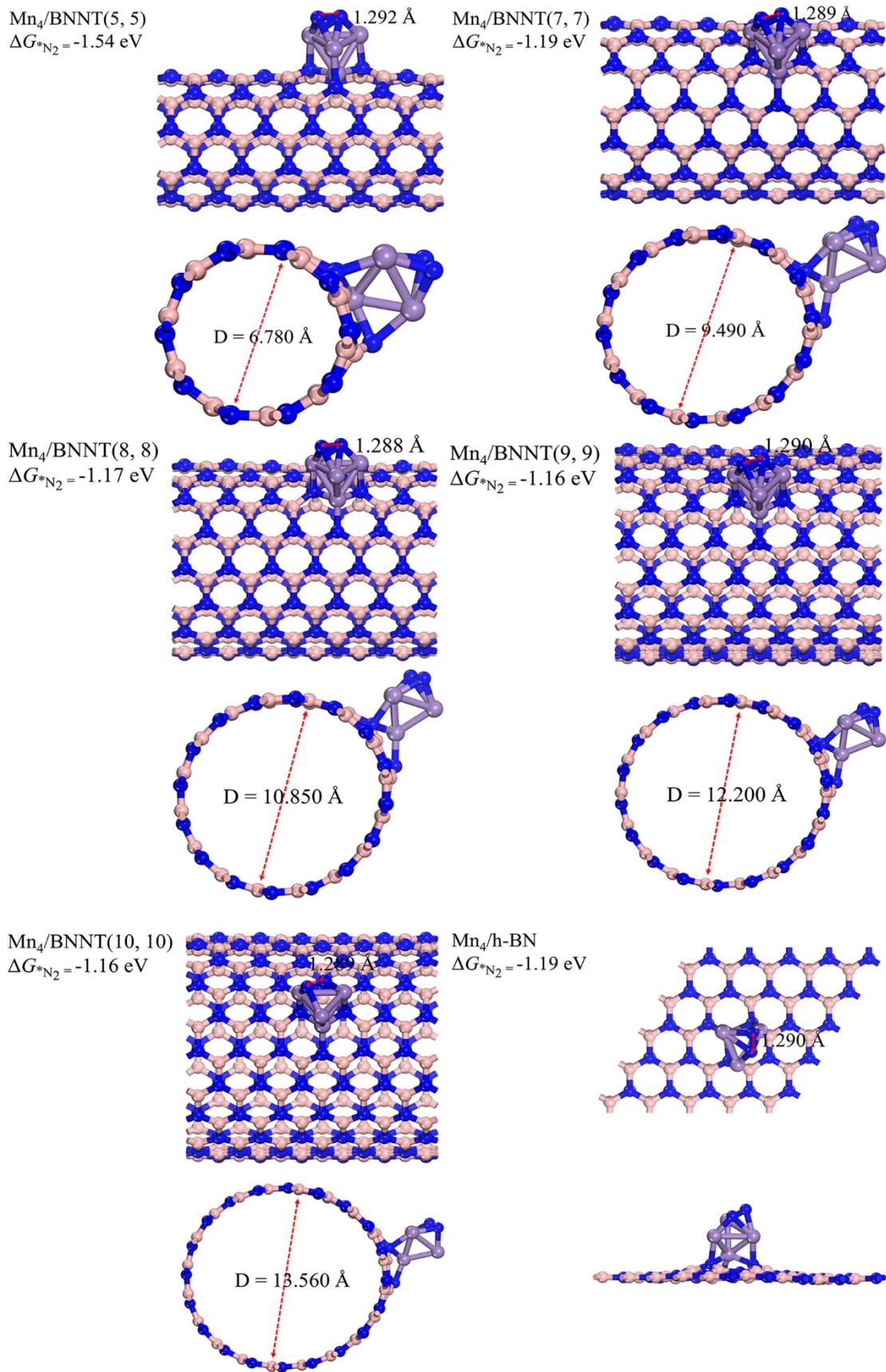
Fig. S5 Atomic structures for N$_2$ adsorbed on BNNT (n, n) with different armchair chirality and h-

BN monolayer. The bond length and $\Delta G_{N_2^*}$ are presented for each system.
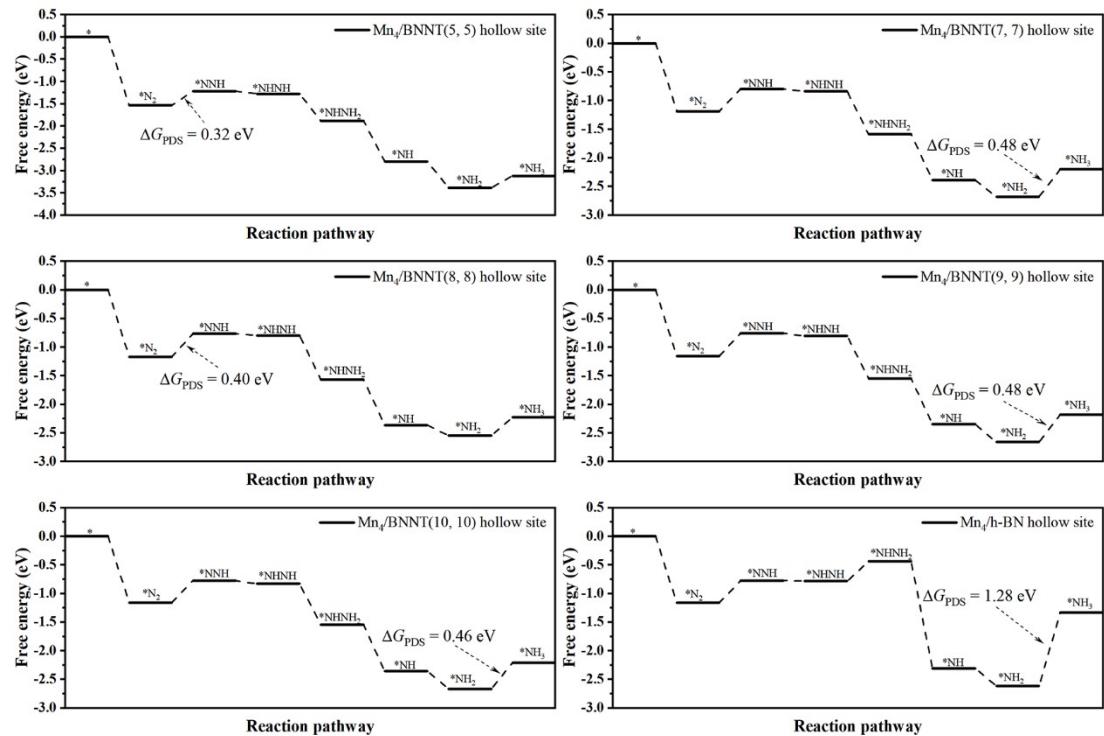
Fig. S6 Reaction pathway of NRR on Mn$_4$/BNNT with armchair chirality including (5, 5), (7, 7), (8, 8), (9, 9), (10, 10). The free energy profiles and PDS are shown.
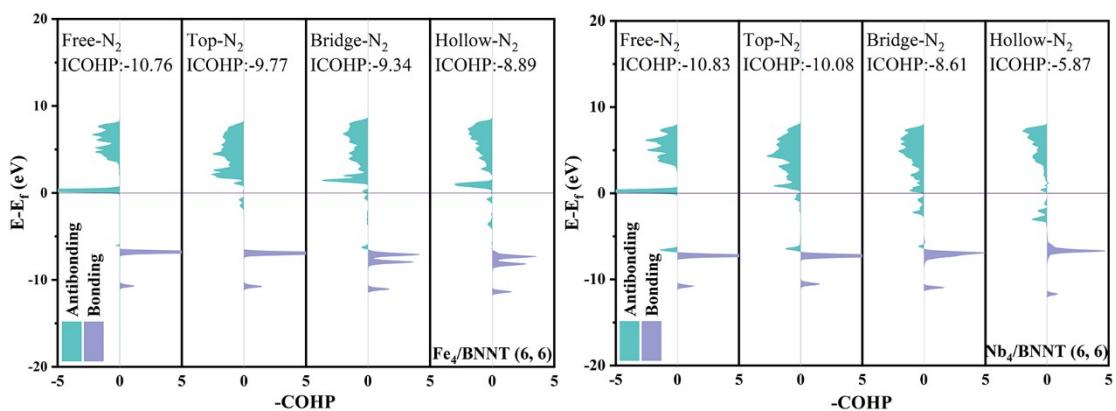
Fig. S7 Analysis of crystal orbital Hamilton population (COHP) and their integration (ICOHP) of N_2 on different site of Fe_4/BNNT (6, 6) and Nb_4/BNNT (6, 6).
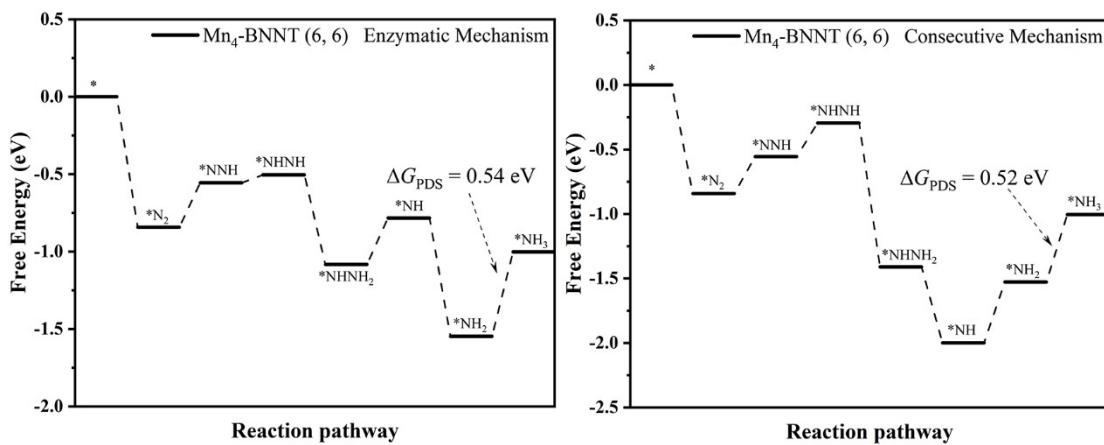
Fig. S8 NRR reaction pathway of Mn_4/BNNT (6, 6) via enzymatic and consecutive mechanism. The free energy profiles and the potential determining step (PDS) are shown.
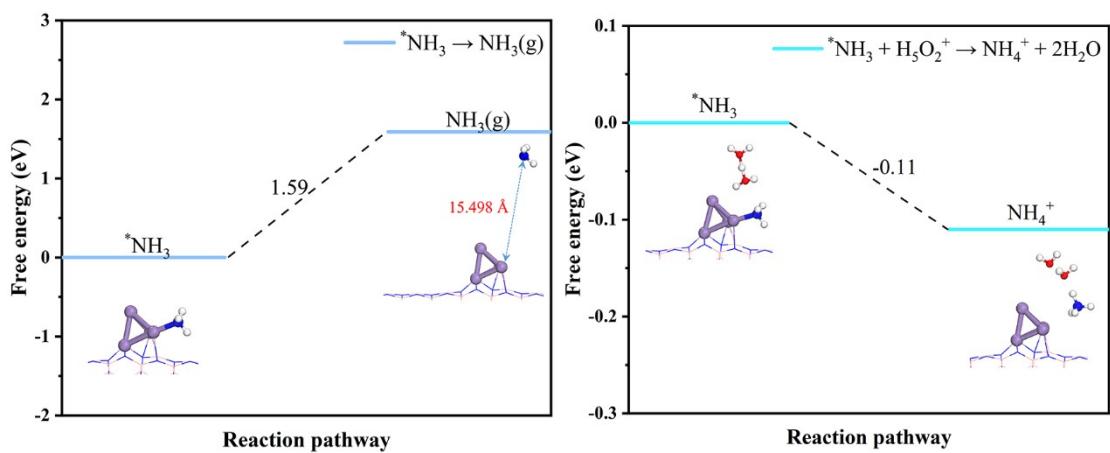
Fig. S9 Reaction pathway of $^*NH_3$ desorption and NH_4^+ formation on Mn_4/BNNT (6, 6). The protons come from $H_5O_2^+$. The solvation model is used with a dielectric constant of 78.54.
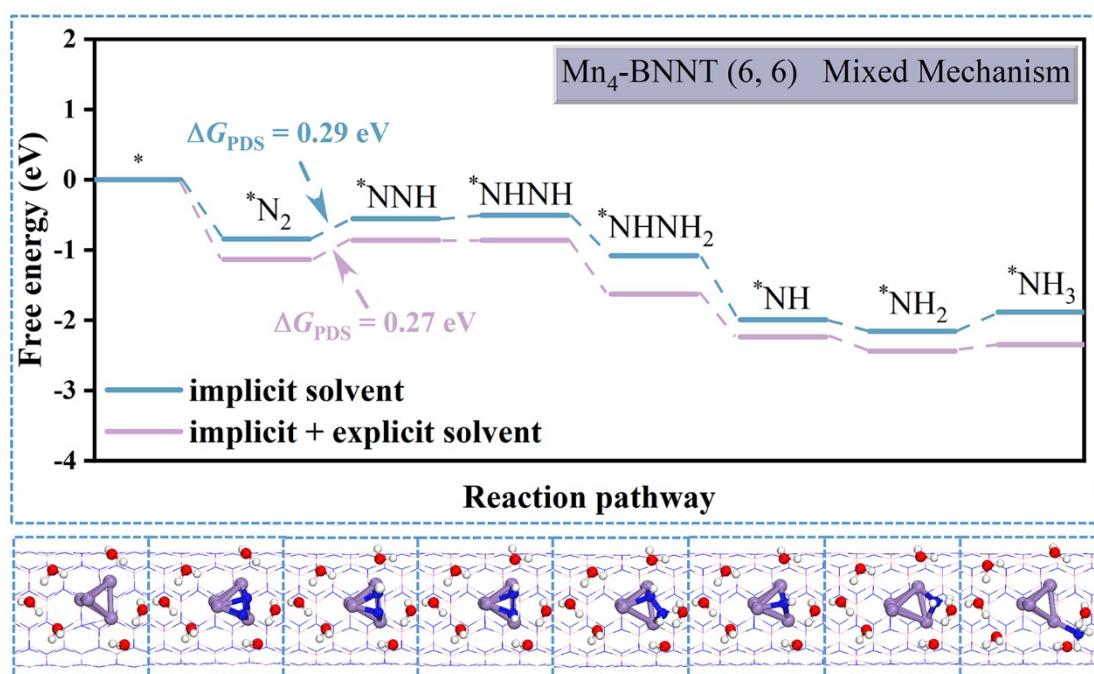
Fig. S10 Comparison between implicit solvent and ″implicit + explicit″ solvent.
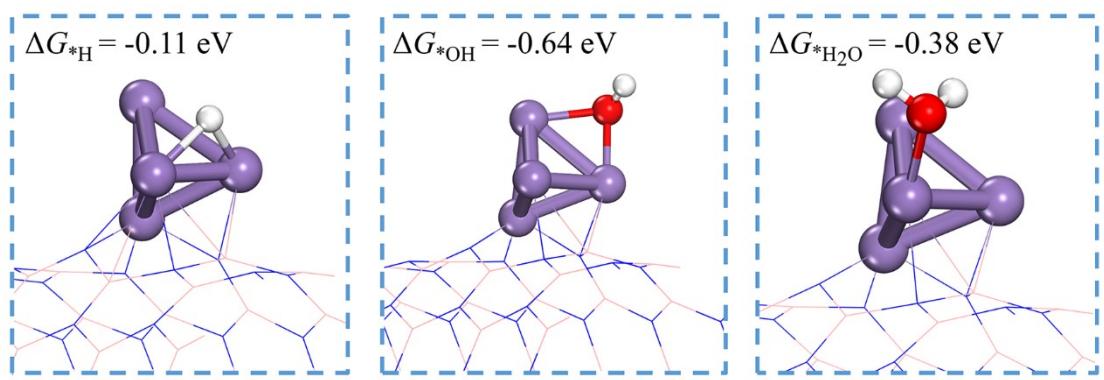
Fig. S11 Adsorption configurations of *H, *OH and *H$_2$O on the Mn$_4$/BNNT (6, 6) and corresponding adsorption free energy.
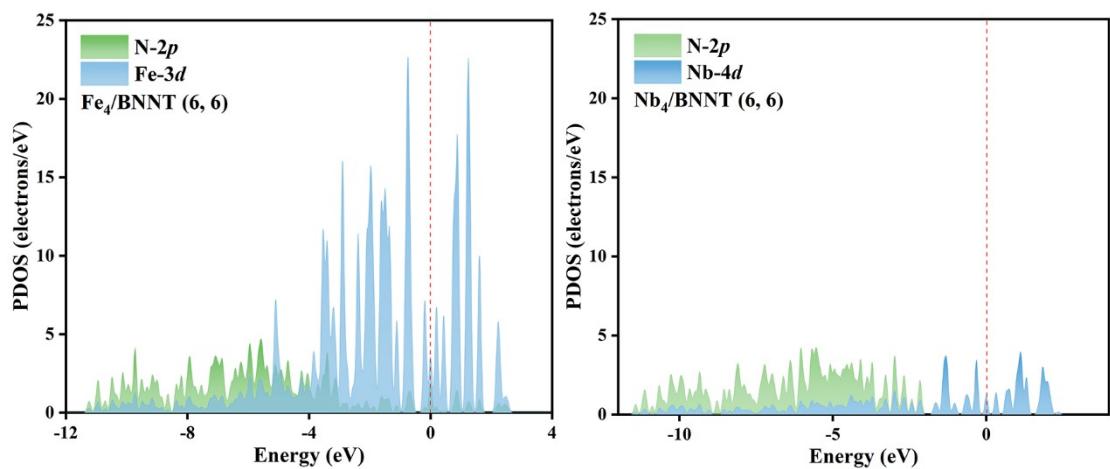
Fig. S12 Partial density of states (PDOS) of Fe$_4$/BNNT (6, 6) and Nb$_4$/BNNT (6, 6), including the Fe-3d (Nb-4d) orbital and adjacent N-2p orbital. The fermi energy level is set to zero.
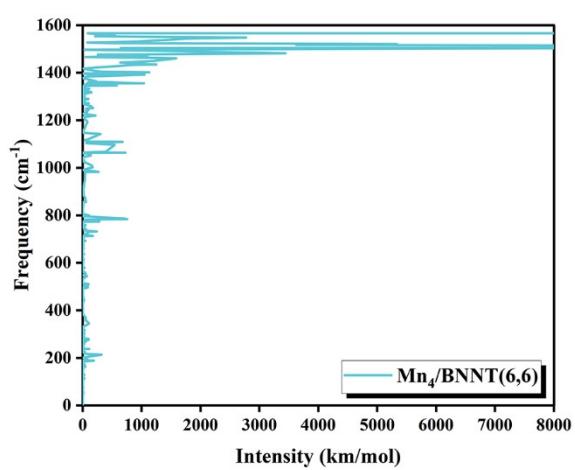
Fig. S13 Frequency distribution of Mn$_4$/BNNT (6, 6) after optimization.
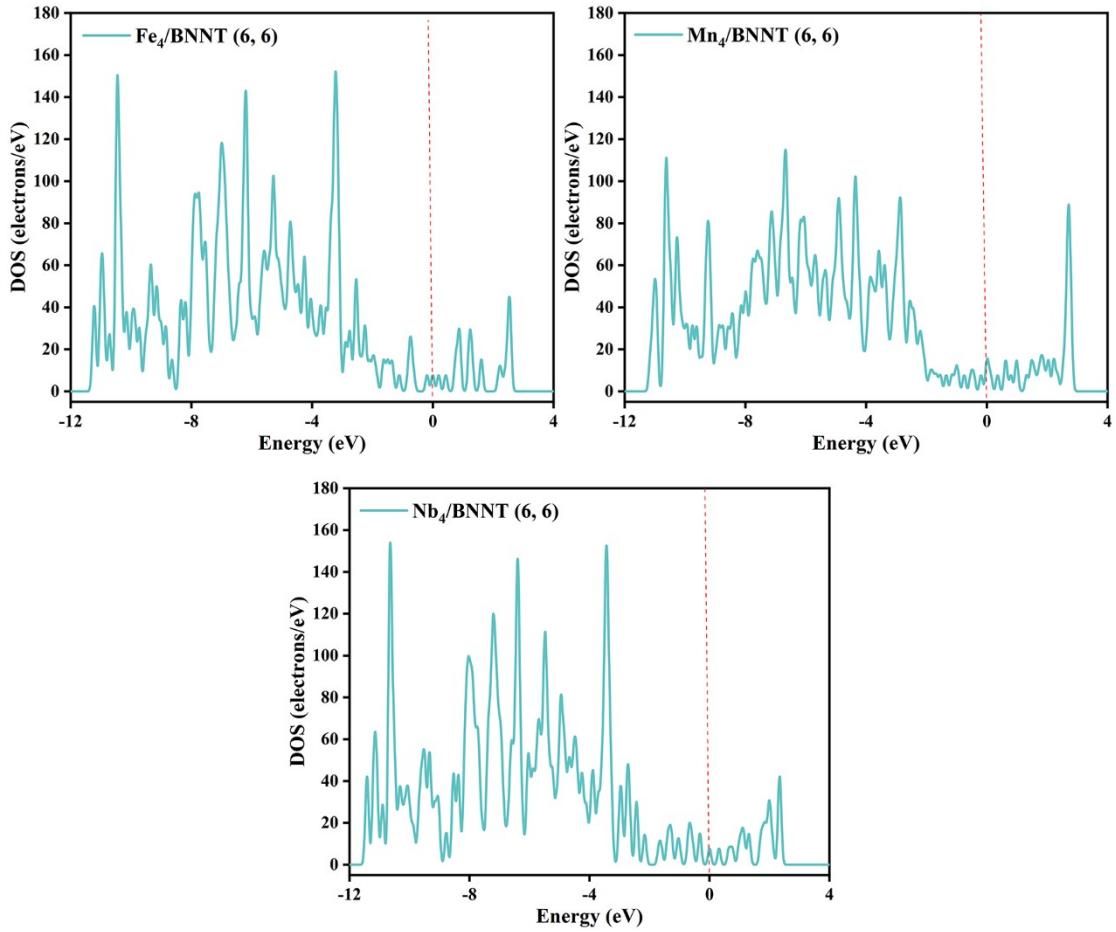
Fig. S14 Density of states (DOS) of TM_4/BNNT (6, 6) (TM = Fe, Mn, Nb). The fermi energy level is set to zero, which is the red dashed line.

Table S1 The formation energy of B-vacancy and N-vacancy on BNNT (n, n).

system	B-vacancy (eV)	N-vacancy (eV)
BNNT (5, 5)	8.28	11.68
BNNT (6, 6)	8.34	11.89
BNNT (7, 7)	8.65	11.90
BNNT (8, 8)	8.70	11.94
BNNT (9, 9)	8.80	12.02
BNNT (10, 10)	8.83	12.12

Table S2 Corresponding ΔG of *N$_2$ Adsorbed on B or N Sites of TM$_4$/BNNT (6, 6)

(TM = Fe, Mn, Nb). *

system	N$_2$		H$^+$	
	B-site	N-site	B-site	N-site
Fe$_4$/BNNT (6,6)	1.41	0.66	2.57	2.76
Mn$_4$/BNNT (6,6)	1.14	0.96	2.15	3.01
Nb$_4$/BNNT (6,6)	0.88	1.07	1.87	3.46

*The values are given in units of eV.

Note S1. Geometrical coordinates of calculation models

The factional coordinates of all the models in this manuscript are listed below, including TM$_4$ clusters decorated on BNNTs with various tube diameters and Mn$_4$ adsorbed on h-BN (0001), as well as the key reaction intermediates adsorbed on Mn$_4$/BNNT (6, 6). Additionally, the cell parameters and DFT total energy corresponding to each model are also displayed at the beginning, where the cell parameters and energy are given in the unit of angstrom and electron volt, respectively.

(1)　　Mn$_4$/BNNT (5, 5) ($G = -142626.6212$ eV)

1.0

25.1270008087	0.0000000000	0.0000000000
-12.5635004044	21.7606210213	0.0000000000
0.0000000000	0.0000000000	14.7571001053

N	B	Mn
60	59	4

Direct

0.365630000	0.287440000	0.072730000
0.245820000	0.357980000	0.069040000
0.328280000	0.349830000	0.151340000
0.145680000	0.306140000	0.153690000
0.064700000	0.213410000	0.070710000
0.069400000	0.049960000	0.071210000
0.035350000	0.115010000	0.154250000
0.153190000	0.043710000	0.155200000
0.254400000	0.097330000	0.072900000
0.334180000	0.190810000	0.156980000
0.368650000	0.291440000	0.243110000
0.246940000	0.360680000	0.235730000
0.342470000	0.375100000	0.308950000
0.147560000	0.305460000	0.320630000

0.065590000	0.213300000	0.237470000
0.068790000	0.049290000	0.237950000
0.035020000	0.114560000	0.320890000
0.153090000	0.043780000	0.321970000
0.253470000	0.097950000	0.239170000
0.335260000	0.190250000	0.322340000
0.407610000	0.288060000	0.406640000
0.249810000	0.359130000	0.403050000
0.336630000	0.358540000	0.492950000
0.147820000	0.304670000	0.486350000
0.065840000	0.212960000	0.403750000
0.068660000	0.049130000	0.404810000
0.034910000	0.114500000	0.487640000
0.153570000	0.044210000	0.488430000
0.254330000	0.097820000	0.405330000
0.338380000	0.187990000	0.489230000
0.371020000	0.287230000	0.570060000
0.247260000	0.355360000	0.570440000
0.330140000	0.347450000	0.655320000
0.146060000	0.305170000	0.653150000
0.065130000	0.213040000	0.570170000
0.069340000	0.049760000	0.571570000
0.035100000	0.114850000	0.654340000
0.153980000	0.044390000	0.655160000
0.254450000	0.096750000	0.571850000
0.337140000	0.187810000	0.655470000
0.366570000	0.285500000	0.738570000
0.246390000	0.355310000	0.736640000
0.329800000	0.349100000	0.820960000
0.145290000	0.305750000	0.819820000

0.064280000	0.213170000	0.736980000
0.069960000	0.050420000	0.738180000
0.035330000	0.115170000	0.821000000
0.154280000	0.044620000	0.821880000
0.255010000	0.096060000	0.738760000
0.337230000	0.187680000	0.822680000
0.366040000	0.286210000	0.905510000
0.245920000	0.356850000	0.902830000
0.329140000	0.349860000	0.986380000
0.144980000	0.306250000	0.986610000
0.064230000	0.213360000	0.903840000
0.070040000	0.050550000	0.904680000
0.035440000	0.115250000	0.987620000
0.153990000	0.044410000	0.988590000
0.255030000	0.096200000	0.905930000
0.336520000	0.188650000	0.989830000
0.344510000	0.331410000	0.069480000
0.179090000	0.327070000	0.069790000
0.276360000	0.360210000	0.152170000
0.090070000	0.246240000	0.154010000
0.041530000	0.147480000	0.070960000
0.122900000	0.041990000	0.071630000
0.053850000	0.068600000	0.154540000
0.219950000	0.076220000	0.155750000
0.310290000	0.157090000	0.073550000
0.358790000	0.256880000	0.158450000
0.350450000	0.340170000	0.235750000
0.180230000	0.327230000	0.236670000
0.281300000	0.368050000	0.317370000
0.091260000	0.245990000	0.320720000

0.041670000	0.147250000	0.237650000
0.122420000	0.041540000	0.238460000
0.053450000	0.068120000	0.321300000
0.219920000	0.076500000	0.322460000
0.308580000	0.157890000	0.239820000
0.373070000	0.257140000	0.324390000
0.182500000	0.326200000	0.403390000
0.279830000	0.360430000	0.487730000
0.091160000	0.245680000	0.486830000
0.041510000	0.146910000	0.404170000
0.122480000	0.041670000	0.405230000
0.053620000	0.068280000	0.488090000
0.220450000	0.076210000	0.488510000
0.311580000	0.156740000	0.405630000
0.375480000	0.255310000	0.488610000
0.350230000	0.332760000	0.571710000
0.180760000	0.325150000	0.570220000
0.277140000	0.356160000	0.653920000
0.089830000	0.245840000	0.653500000
0.041320000	0.147050000	0.570750000
0.123100000	0.042180000	0.571830000
0.054190000	0.068890000	0.654750000
0.220780000	0.075660000	0.655310000
0.311280000	0.155570000	0.571850000
0.361310000	0.253850000	0.654350000
0.345900000	0.330000000	0.738730000
0.179740000	0.325690000	0.736610000
0.276570000	0.357470000	0.820190000
0.089250000	0.246140000	0.820250000
0.041190000	0.147280000	0.737470000

0.123530000	0.042540000	0.738500000
0.054540000	0.069300000	0.821340000
0.221090000	0.075490000	0.822240000
0.311700000	0.155180000	0.738940000
0.360430000	0.253560000	0.822310000
0.345580000	0.331100000	0.904240000
0.179160000	0.326540000	0.903140000
0.276200000	0.358670000	0.986120000
0.089280000	0.246330000	0.987120000
0.041320000	0.147490000	0.904210000
0.123550000	0.042580000	0.905070000
0.054360000	0.069170000	0.987880000
0.220820000	0.075830000	0.989180000
0.311550000	0.155420000	0.906310000
0.359950000	0.254530000	0.989680000
0.425650000	0.434690000	0.493660000
0.479330000	0.382180000	0.410600000
0.369350000	0.338930000	0.393530000
0.432970000	0.445790000	0.328140000

(2)　　Mn$_4$/BNNT (6, 6) ($G = -168642.2704$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

　B　　N　　Mn

　71　　72　　4

Direct

0.397010000	0.333200000	0.010040000
0.357260000	0.387150000	0.093050000
0.278810000	0.393630000	0.010480000

0.098710000	0.278440000	0.011180000
0.185170000	0.354040000	0.094400000
0.043140000	0.184530000	0.094560000
0.034080000	0.098860000	0.011370000
0.152240000	0.038140000	0.011770000
0.074150000	0.045100000	0.094900000
0.245890000	0.078380000	0.095670000
0.332190000	0.154790000	0.012980000
0.387470000	0.249280000	0.096920000
0.404380000	0.339670000	0.177390000
0.363120000	0.392490000	0.259600000
0.279450000	0.392620000	0.177440000
0.098830000	0.278060000	0.177790000
0.185570000	0.353290000	0.260980000
0.042860000	0.184320000	0.261180000
0.033710000	0.098550000	0.178050000
0.151880000	0.037970000	0.178680000
0.073880000	0.044940000	0.261730000
0.245880000	0.079040000	0.262470000
0.330650000	0.156060000	0.179460000
0.395400000	0.249370000	0.263440000
0.357460000	0.384220000	0.428210000
0.280150000	0.391580000	0.343850000
0.098630000	0.277940000	0.344220000
0.185230000	0.353380000	0.427070000
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0.033550000	0.098520000	0.344820000
0.152030000	0.038420000	0.345450000
0.074110000	0.045290000	0.428510000
0.246510000	0.079270000	0.428620000

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0.400100000	0.248050000	0.427790000
0.398820000	0.331740000	0.511510000
0.354280000	0.381990000	0.594230000
0.278140000	0.391070000	0.510680000
0.098460000	0.278330000	0.510800000
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0.033790000	0.098820000	0.511560000
0.152620000	0.039070000	0.511960000
0.074640000	0.045800000	0.595130000
0.246980000	0.078870000	0.595140000
0.333940000	0.154640000	0.511570000
0.391610000	0.247340000	0.594670000
0.396390000	0.330630000	0.678610000
0.355280000	0.384200000	0.760480000
0.278050000	0.392430000	0.677150000
0.098290000	0.278670000	0.677620000
0.184390000	0.354930000	0.760730000
0.043230000	0.184900000	0.761270000
0.034160000	0.099130000	0.678190000
0.152970000	0.039180000	0.678500000
0.074910000	0.045970000	0.761650000
0.247090000	0.078090000	0.761960000
0.334230000	0.153600000	0.678640000
0.389940000	0.246780000	0.762250000
0.396950000	0.332120000	0.844330000
0.356140000	0.385860000	0.926650000
0.278380000	0.393450000	0.843750000
0.098460000	0.278690000	0.844440000

0.184690000	0.354850000	0.927590000
0.043290000	0.184800000	0.927940000
0.034290000	0.099140000	0.844770000
0.152850000	0.038800000	0.845080000
0.074660000	0.045620000	0.928180000
0.246650000	0.077960000	0.928920000
0.333620000	0.153490000	0.845930000
0.388900000	0.247480000	0.929220000
0.391920000	0.358730000	0.092320000
0.335160000	0.396810000	0.009960000
0.152900000	0.333970000	0.011120000
0.248490000	0.386860000	0.094310000
0.073670000	0.247850000	0.094420000
0.032000000	0.152660000	0.011200000
0.095860000	0.034970000	0.011580000
0.039680000	0.073900000	0.094700000
0.182620000	0.044140000	0.095360000
0.278230000	0.099070000	0.012630000
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0.356100000	0.186070000	0.096270000
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0.248940000	0.385560000	0.260940000
0.073470000	0.247620000	0.260970000
0.031690000	0.152380000	0.177850000
0.095390000	0.034570000	0.178400000
0.039340000	0.073690000	0.261490000
0.182610000	0.044560000	0.262150000
0.277420000	0.100040000	0.179060000

0.400790000	0.282210000	0.180880000
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0.393830000	0.358960000	0.431920000
0.337680000	0.396650000	0.343630000
0.153170000	0.333000000	0.343930000
0.248460000	0.385160000	0.426620000
0.073330000	0.247750000	0.427620000
0.031500000	0.152340000	0.344600000
0.095410000	0.034740000	0.345200000
0.039420000	0.073860000	0.428290000
0.183140000	0.045320000	0.428590000
0.278230000	0.100310000	0.345340000
0.426350000	0.279260000	0.344520000
0.360190000	0.184760000	0.428510000
0.388290000	0.352950000	0.595490000
0.333200000	0.392420000	0.510930000
0.152740000	0.333690000	0.510400000
0.247670000	0.386690000	0.593770000
0.073320000	0.248090000	0.594330000
0.031670000	0.152600000	0.511360000
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0.152280000	0.334350000	0.677390000
0.247730000	0.387550000	0.760560000

0.073420000	0.248230000	0.761110000
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0.096490000	0.035790000	0.678390000
0.040160000	0.074450000	0.761500000
0.183690000	0.045240000	0.761820000
0.279140000	0.098760000	0.678570000
0.401540000	0.278560000	0.678850000
0.359470000	0.183390000	0.762530000
0.390770000	0.357270000	0.926760000
0.334310000	0.395640000	0.843510000
0.152480000	0.334390000	0.844320000
0.248050000	0.387880000	0.927360000
0.073600000	0.248130000	0.927820000
0.032110000	0.152890000	0.844610000
0.096450000	0.035630000	0.844930000
0.040060000	0.074270000	0.928040000
0.183270000	0.044650000	0.928610000
0.278940000	0.098320000	0.845690000
0.400440000	0.279030000	0.845440000
0.358260000	0.184170000	0.929490000
0.498110000	0.416660000	0.217080000
0.553620000	0.438690000	0.363430000
0.451400000	0.366830000	0.351770000
0.512270000	0.331570000	0.290250000

(3)   Mn$_4$/BNNT (7, 7) ($G = -194655.7682$ eV)

1.0

27.8390007019	0.0000000000	0.0000000000
-13.9195003510	24.1092818238	0.0000000000
0.0000000000	0.0000000000	14.7571001053

N   B   Mn

84   83   4
Direct

0.437870000	0.347400000	0.033060000
0.343640000	0.429780000	0.033370000
0.408930000	0.407110000	0.114860000
0.258290000	0.412370000	0.117460000
0.167440000	0.363290000	0.033970000
0.034840000	0.195250000	0.033380000
0.087400000	0.285570000	0.116970000
0.021850000	0.110830000	0.116740000
0.051360000	0.051120000	0.033410000
0.201170000	0.043440000	0.033260000
0.115660000	0.027590000	0.116680000
0.291700000	0.094180000	0.116670000
0.371090000	0.172560000	0.033580000
0.422930000	0.263300000	0.117000000
0.440370000	0.350030000	0.201050000
0.344130000	0.428310000	0.200060000
0.422210000	0.424160000	0.275880000
0.259010000	0.410290000	0.284220000
0.167960000	0.361970000	0.200760000
0.034060000	0.194910000	0.200060000
0.087280000	0.285140000	0.283610000
0.021620000	0.110730000	0.283460000
0.051510000	0.051320000	0.200110000
0.200910000	0.042870000	0.199920000
0.115580000	0.027450000	0.283340000
0.291480000	0.094110000	0.283310000
0.369990000	0.172990000	0.200190000
0.423550000	0.263680000	0.283140000

0.461040000	0.353990000	0.366600000
0.347100000	0.430480000	0.366970000
0.423020000	0.425460000	0.457840000
0.259090000	0.410640000	0.449740000
0.168170000	0.361370000	0.366970000
0.033740000	0.194760000	0.366890000
0.087370000	0.285210000	0.450230000
0.021700000	0.110760000	0.450190000
0.051640000	0.051440000	0.366760000
0.200760000	0.042420000	0.366590000
0.115620000	0.027440000	0.450020000
0.291460000	0.093990000	0.449790000
0.370020000	0.173250000	0.366610000
0.422940000	0.263730000	0.450100000
0.439900000	0.350230000	0.532110000
0.344510000	0.429350000	0.533790000
0.408830000	0.407470000	0.618720000
0.258450000	0.413050000	0.616510000
0.168060000	0.362230000	0.533190000
0.034280000	0.194990000	0.533670000
0.087640000	0.285680000	0.616830000
0.021980000	0.110880000	0.616870000
0.051590000	0.051330000	0.533400000
0.200910000	0.042740000	0.533300000
0.115730000	0.027590000	0.616710000
0.291700000	0.094020000	0.616480000
0.369800000	0.172980000	0.532990000
0.422290000	0.263340000	0.616120000
0.437420000	0.347370000	0.700130000
0.343710000	0.430250000	0.700620000

0.407680000	0.406690000	0.784150000
0.258160000	0.414740000	0.783560000
0.167550000	0.363620000	0.699980000
0.035040000	0.195330000	0.700270000
0.087800000	0.285990000	0.783500000
0.022160000	0.110980000	0.783490000
0.051430000	0.051140000	0.700100000
0.201180000	0.043340000	0.700010000
0.115780000	0.027720000	0.783380000
0.292040000	0.094260000	0.783190000
0.370990000	0.172570000	0.699560000
0.424330000	0.262750000	0.783090000
0.437600000	0.347140000	0.866590000
0.343580000	0.430580000	0.867020000
0.407850000	0.406690000	0.949480000
0.258100000	0.414430000	0.950570000
0.167340000	0.364010000	0.866990000
0.035270000	0.195430000	0.866800000
0.087670000	0.285930000	0.950210000
0.022100000	0.110960000	0.950090000
0.051310000	0.051040000	0.866760000
0.201340000	0.043760000	0.866640000
0.115750000	0.027720000	0.950020000
0.292020000	0.094360000	0.949990000
0.371660000	0.172200000	0.866570000
0.424520000	0.262740000	0.949970000
0.420740000	0.388540000	0.032070000
0.287810000	0.421320000	0.033710000
0.367520000	0.424000000	0.115900000
0.198100000	0.381320000	0.117340000

0.113260000	0.313210000	0.033750000
0.023610000	0.138330000	0.033410000
0.050100000	0.225890000	0.116850000
0.038890000	0.069270000	0.116730000
0.092180000	0.033100000	0.033370000
0.261450000	0.075140000	0.033250000
0.171370000	0.035480000	0.116590000
0.345190000	0.145050000	0.116880000
0.408090000	0.232320000	0.033760000
0.435720000	0.320680000	0.117700000
0.426190000	0.393750000	0.198730000
0.288120000	0.419000000	0.200370000
0.372060000	0.428280000	0.282480000
0.198750000	0.379920000	0.283970000
0.113350000	0.312570000	0.200470000
0.023140000	0.138100000	0.200080000
0.049610000	0.225550000	0.283540000
0.038940000	0.069380000	0.283450000
0.092180000	0.033090000	0.200050000
0.261190000	0.074860000	0.199950000
0.171180000	0.035060000	0.283270000
0.344800000	0.145280000	0.283500000
0.406910000	0.232710000	0.200550000
0.443950000	0.323510000	0.284600000
0.289580000	0.418890000	0.366990000
0.372530000	0.429150000	0.451490000
0.198810000	0.380130000	0.449960000
0.113390000	0.312250000	0.366900000
0.022980000	0.138010000	0.366840000
0.049730000	0.225620000	0.450220000

0.038990000	0.069400000	0.450110000
0.092220000	0.033090000	0.366710000
0.261060000	0.074580000	0.366540000
0.171200000	0.035010000	0.449960000
0.344720000	0.145240000	0.449650000
0.407660000	0.233170000	0.366630000
0.443510000	0.323610000	0.448640000
0.426250000	0.394370000	0.534700000
0.288340000	0.419720000	0.533570000
0.367690000	0.424710000	0.617970000
0.198230000	0.381750000	0.616610000
0.113510000	0.312710000	0.533350000
0.023290000	0.138160000	0.533570000
0.050350000	0.225990000	0.616860000
0.038980000	0.069290000	0.616780000
0.092250000	0.033090000	0.533360000
0.261190000	0.074710000	0.533190000
0.171410000	0.035410000	0.616680000
0.345110000	0.145000000	0.616300000
0.406370000	0.232740000	0.532630000
0.435130000	0.320720000	0.615390000
0.420460000	0.388630000	0.701360000
0.287910000	0.421870000	0.700340000
0.367110000	0.424860000	0.784010000
0.197860000	0.382980000	0.783530000
0.113460000	0.313390000	0.700050000
0.023760000	0.138390000	0.700200000
0.050800000	0.226250000	0.783500000
0.038890000	0.069200000	0.783440000
0.092240000	0.033100000	0.700040000

0.261460000	0.075000000	0.699930000
0.171590000	0.035850000	0.783340000
0.345920000	0.144770000	0.783070000
0.407790000	0.232360000	0.699330000
0.435730000	0.319630000	0.783140000
0.420430000	0.388490000	0.866730000
0.287810000	0.422460000	0.867060000
0.367140000	0.424690000	0.949870000
0.197810000	0.382760000	0.950520000
0.113380000	0.313600000	0.866900000
0.023890000	0.138470000	0.866790000
0.050680000	0.226180000	0.950150000
0.038850000	0.069200000	0.950080000
0.092200000	0.033110000	0.866700000
0.261630000	0.075280000	0.866600000
0.171560000	0.035870000	0.949940000
0.345930000	0.144790000	0.950090000
0.408850000	0.231900000	0.866540000
0.435970000	0.319650000	0.949950000
0.567710000	0.506920000	0.360730000
0.484920000	0.510020000	0.278250000
0.472120000	0.427310000	0.366420000
0.487220000	0.511030000	0.452250000

(4) Mn_4/BNNT (8, 8) ($G = -220669.4141$ eV)

1.0

29.1949996948	0.0000000000	0.0000000000
-14.5974998474	25.2836113992	0.0000000000
0.0000000000	0.0000000000	14.7571001053

N   B   Mn

96   95   4

Direct

0.460610000	0.407930000	0.054750000
0.419870000	0.453400000	0.136520000
0.350840000	0.464720000	0.054660000
0.181100000	0.392080000	0.055240000
0.267570000	0.441480000	0.138750000
0.103810000	0.319140000	0.138330000
0.046900000	0.234200000	0.054820000
0.026340000	0.077740000	0.054890000
0.019580000	0.149220000	0.138150000
0.066940000	0.031730000	0.138250000
0.134360000	0.018260000	0.054880000
0.303950000	0.091060000	0.054840000
0.217740000	0.039310000	0.138160000
0.379790000	0.165080000	0.138300000
0.436220000	0.250450000	0.055160000
0.463980000	0.335610000	0.138620000
0.462910000	0.410850000	0.222760000
0.431960000	0.471800000	0.297170000
0.351690000	0.463940000	0.221450000
0.181710000	0.390650000	0.222040000
0.268420000	0.439390000	0.305520000
0.103680000	0.318760000	0.304960000
0.046370000	0.233980000	0.221480000
0.026300000	0.077740000	0.221560000
0.019250000	0.149080000	0.304860000
0.067020000	0.031840000	0.304910000
0.134370000	0.018240000	0.221550000
0.303860000	0.090760000	0.221530000
0.217680000	0.039060000	0.304860000

0.379520000	0.165090000	0.304970000
0.434850000	0.250420000	0.221760000
0.465090000	0.336170000	0.304710000
0.483790000	0.418530000	0.388210000
0.432090000	0.472190000	0.479430000
0.354470000	0.466220000	0.388270000
0.181940000	0.389880000	0.388260000
0.268420000	0.439440000	0.471020000
0.103670000	0.318770000	0.471560000
0.046090000	0.233870000	0.388250000
0.026270000	0.077750000	0.388240000
0.019250000	0.149080000	0.471630000
0.067020000	0.031840000	0.471550000
0.134370000	0.018220000	0.388220000
0.303820000	0.090560000	0.388200000
0.217670000	0.039050000	0.471570000
0.379510000	0.165080000	0.471430000
0.435160000	0.250690000	0.388200000
0.464940000	0.336140000	0.471700000
0.462680000	0.410810000	0.553590000
0.419810000	0.453480000	0.639970000
0.351720000	0.464160000	0.555090000
0.181710000	0.390680000	0.554480000
0.267570000	0.441560000	0.637790000
0.103810000	0.319150000	0.638190000
0.046370000	0.233980000	0.555030000
0.026290000	0.077740000	0.554920000
0.019580000	0.149220000	0.638340000
0.066950000	0.031740000	0.638210000
0.134370000	0.018240000	0.554900000

0.303860000	0.090740000	0.554880000
0.217740000	0.039300000	0.638270000
0.379770000	0.165060000	0.638100000
0.434760000	0.250410000	0.554640000
0.463760000	0.335570000	0.637760000
0.460480000	0.407900000	0.721640000
0.418760000	0.452700000	0.805520000
0.350860000	0.464870000	0.721900000
0.181100000	0.392100000	0.721300000
0.267210000	0.443550000	0.804780000
0.103900000	0.319460000	0.804900000
0.046900000	0.234210000	0.721680000
0.026340000	0.077740000	0.721580000
0.019900000	0.149370000	0.804950000
0.066870000	0.031630000	0.804890000
0.134360000	0.018260000	0.721560000
0.303940000	0.091040000	0.721580000
0.217800000	0.039540000	0.804920000
0.380210000	0.165170000	0.804800000
0.436150000	0.250440000	0.721220000
0.465930000	0.335620000	0.804750000
0.460640000	0.407780000	0.888190000
0.418770000	0.452670000	0.970970000
0.350730000	0.465390000	0.888280000
0.180890000	0.392670000	0.888270000
0.267210000	0.443500000	0.971780000
0.103900000	0.319450000	0.971610000
0.047150000	0.234300000	0.888250000
0.026370000	0.077740000	0.888240000
0.019900000	0.149370000	0.971530000

0.066860000	0.031620000	0.971570000
0.134350000	0.018270000	0.888220000
0.304000000	0.091270000	0.888210000
0.217800000	0.039540000	0.971520000
0.380220000	0.165180000	0.971600000
0.437120000	0.250360000	0.888190000
0.466000000	0.335630000	0.971610000
0.435010000	0.439370000	0.053730000
0.464140000	0.385440000	0.139430000
0.375650000	0.462690000	0.137310000
0.296060000	0.452100000	0.054950000
0.128980000	0.344940000	0.055080000
0.210260000	0.409810000	0.138600000
0.064340000	0.263200000	0.138250000
0.026830000	0.177530000	0.054850000
0.051290000	0.045340000	0.054900000
0.021930000	0.100660000	0.138200000
0.110290000	0.020700000	0.138230000
0.189030000	0.030150000	0.054850000
0.355370000	0.139120000	0.054880000
0.275090000	0.071850000	0.138160000
0.418160000	0.221330000	0.138460000
0.457170000	0.307300000	0.055410000
0.440520000	0.445680000	0.220330000
0.472590000	0.389730000	0.306150000
0.380220000	0.468030000	0.303760000
0.296620000	0.449970000	0.221680000
0.129130000	0.344290000	0.221810000
0.210980000	0.408280000	0.305250000
0.063950000	0.262960000	0.304920000

0.026390000	0.177330000	0.221510000
0.051340000	0.045430000	0.221570000
0.021800000	0.100610000	0.304890000
0.110320000	0.020730000	0.304900000
0.188980000	0.029970000	0.221520000
0.355110000	0.139010000	0.221620000
0.275020000	0.071570000	0.304860000
0.417750000	0.221440000	0.305130000
0.455920000	0.307260000	0.222100000
0.472450000	0.389680000	0.470220000
0.380250000	0.468230000	0.472890000
0.298000000	0.449700000	0.388270000
0.129150000	0.343920000	0.388260000
0.210970000	0.408300000	0.471270000
0.063950000	0.262960000	0.471590000
0.026160000	0.177220000	0.388250000
0.051370000	0.045480000	0.388230000
0.021790000	0.100610000	0.471600000
0.110320000	0.020730000	0.471560000
0.188950000	0.029870000	0.388220000
0.355010000	0.138900000	0.388200000
0.275020000	0.071570000	0.471560000
0.417720000	0.221430000	0.471260000
0.457130000	0.307910000	0.388200000
0.440420000	0.445740000	0.556110000
0.463920000	0.385390000	0.636900000
0.375670000	0.462860000	0.639250000
0.296610000	0.450090000	0.554860000
0.129130000	0.344300000	0.554710000
0.210250000	0.409850000	0.637930000

0.064340000	0.263210000	0.638260000
0.026390000	0.177330000	0.554990000
0.051340000	0.045430000	0.554890000
0.021930000	0.100660000	0.638280000
0.110290000	0.020700000	0.638220000
0.188980000	0.029960000	0.554910000
0.355100000	0.138990000	0.554780000
0.275090000	0.071830000	0.638260000
0.418100000	0.221320000	0.637940000
0.455760000	0.307220000	0.554290000
0.434940000	0.439390000	0.722720000
0.464610000	0.384620000	0.804730000
0.375090000	0.463030000	0.805330000
0.296060000	0.452200000	0.721610000
0.128980000	0.344950000	0.721440000
0.209840000	0.411270000	0.804800000
0.064690000	0.263410000	0.804930000
0.026820000	0.177530000	0.721640000
0.051290000	0.045340000	0.721560000
0.022060000	0.100700000	0.804930000
0.110260000	0.020660000	0.804890000
0.189030000	0.030150000	0.721580000
0.355360000	0.139100000	0.721530000
0.275140000	0.072100000	0.804920000
0.419180000	0.221330000	0.804700000
0.457050000	0.307280000	0.720960000
0.434920000	0.439350000	0.888220000
0.464680000	0.384630000	0.971620000
0.375090000	0.462970000	0.971210000
0.295970000	0.453090000	0.888280000

0.128940000	0.345230000	0.888260000
0.209840000	0.411250000	0.971750000
0.064690000	0.263410000	0.971580000
0.027030000	0.177620000	0.888250000
0.051260000	0.045290000	0.888230000
0.022060000	0.100710000	0.971550000
0.110260000	0.020660000	0.971560000
0.189040000	0.030240000	0.888220000
0.355530000	0.139220000	0.888210000
0.275140000	0.072110000	0.971510000
0.419210000	0.221330000	0.971690000
0.458320000	0.307220000	0.888180000
0.483600000	0.556760000	0.475260000
0.482470000	0.556500000	0.301090000
0.567760000	0.566110000	0.385260000
0.482280000	0.482820000	0.388270000

(5)　　Mn$_4$/BNNT (9, 9) ($G = -246682.8678$ eV)

1.0

30.5510005951	0.0000000000	0.0000000000
-15.2755002975	26.4579426264	0.0000000000
0.0000000000	0.0000000000	14.7571001053

　B　　N　　Mn

　107　　108　　4

Direct

0.498170000	0.376290000	0.077300000
0.482560000	0.438140000	0.159420000
0.438860000	0.476690000	0.076650000
0.295240000	0.470470000	0.077150000
0.373470000	0.486820000	0.160320000
0.212750000	0.428910000	0.160540000

0.134400000	0.367880000	0.077070000
0.025950000	0.209320000	0.077060000
0.069230000	0.291600000	0.160360000
0.010630000	0.131670000	0.160420000
0.025760000	0.069220000	0.077120000
0.133700000	0.018600000	0.077130000
0.068750000	0.029920000	0.160470000
0.212030000	0.035620000	0.160430000
0.294510000	0.077750000	0.077120000
0.437440000	0.216360000	0.077400000
0.372350000	0.139910000	0.160550000
0.481040000	0.298790000	0.161160000
0.498230000	0.377490000	0.245160000
0.489340000	0.444440000	0.326040000
0.439410000	0.476600000	0.242770000
0.295160000	0.468700000	0.243980000
0.373530000	0.484920000	0.327050000
0.212800000	0.427880000	0.327280000
0.134240000	0.367670000	0.243770000
0.025770000	0.209280000	0.243690000
0.068870000	0.291530000	0.327010000
0.010610000	0.131700000	0.327080000
0.025840000	0.069290000	0.243800000
0.133670000	0.018480000	0.243790000
0.068830000	0.029980000	0.327140000
0.211950000	0.035310000	0.327110000
0.294420000	0.077470000	0.243790000
0.436410000	0.216560000	0.244170000
0.372060000	0.139900000	0.327290000
0.480080000	0.298990000	0.327740000

0.506880000	0.380790000	0.411690000
0.445010000	0.482090000	0.408960000
0.295350000	0.466900000	0.410660000
0.374780000	0.484720000	0.493640000
0.212770000	0.427370000	0.493700000
0.134020000	0.367450000	0.410410000
0.025580000	0.209250000	0.410380000
0.068670000	0.291500000	0.493730000
0.010610000	0.131720000	0.493760000
0.025920000	0.069380000	0.410450000
0.133670000	0.018410000	0.410470000
0.068890000	0.030040000	0.493790000
0.211930000	0.035210000	0.493830000
0.294350000	0.077220000	0.410490000
0.436090000	0.216750000	0.410780000
0.371990000	0.139850000	0.493840000
0.481330000	0.299490000	0.493830000
0.506920000	0.380670000	0.576030000
0.489080000	0.443920000	0.661600000
0.444670000	0.481680000	0.578190000
0.295340000	0.466910000	0.576710000
0.373470000	0.484840000	0.660320000
0.212790000	0.427910000	0.660130000
0.134010000	0.367460000	0.577030000
0.025570000	0.209250000	0.577110000
0.068850000	0.291540000	0.660450000
0.010620000	0.131710000	0.660440000
0.025940000	0.069400000	0.577100000
0.133700000	0.018470000	0.577150000
0.068870000	0.030050000	0.660440000

0.211990000	0.035420000	0.660530000
0.294370000	0.077250000	0.577190000
0.436220000	0.216720000	0.576910000
0.372140000	0.139900000	0.660400000
0.480350000	0.298930000	0.660000000
0.498360000	0.377360000	0.742640000
0.482640000	0.438100000	0.828170000
0.439270000	0.476340000	0.744620000
0.295150000	0.468730000	0.743410000
0.373450000	0.486780000	0.827050000
0.212740000	0.428930000	0.826860000
0.134220000	0.367690000	0.743670000
0.025750000	0.209290000	0.743800000
0.069210000	0.291610000	0.827110000
0.010630000	0.131680000	0.827110000
0.025860000	0.069330000	0.743760000
0.133730000	0.018600000	0.743820000
0.068790000	0.029990000	0.827110000
0.212070000	0.035730000	0.827200000
0.294460000	0.077540000	0.743880000
0.436630000	0.216500000	0.743570000
0.372430000	0.139900000	0.827150000
0.481280000	0.298750000	0.826640000
0.498250000	0.376270000	0.910430000
0.482610000	0.438170000	0.993780000
0.438860000	0.476660000	0.910750000
0.295230000	0.470490000	0.910240000
0.373660000	0.487840000	0.993680000
0.212740000	0.429380000	0.993710000
0.134390000	0.367890000	0.910370000

0.025940000	0.209320000	0.910440000
0.069390000	0.291640000	0.993730000
0.010630000	0.131660000	0.993760000
0.025780000	0.069240000	0.910430000
0.133730000	0.018660000	0.910470000
0.068730000	0.029920000	0.993790000
0.212080000	0.035820000	0.993810000
0.294530000	0.077790000	0.910530000
0.437540000	0.216330000	0.910360000
0.372590000	0.139950000	0.993850000
0.482080000	0.298480000	0.993900000
0.498050000	0.400630000	0.160430000
0.471730000	0.455240000	0.076540000
0.348670000	0.486150000	0.077150000
0.419830000	0.484730000	0.160040000
0.267560000	0.459600000	0.160670000
0.185090000	0.411620000	0.077100000
0.050800000	0.264140000	0.077020000
0.109630000	0.344040000	0.160340000
0.015890000	0.181630000	0.160380000
0.010940000	0.107580000	0.077100000
0.087550000	0.021330000	0.077120000
0.036210000	0.051950000	0.160470000
0.158600000	0.019960000	0.160440000
0.239770000	0.046230000	0.077120000
0.397030000	0.163870000	0.077280000
0.322020000	0.095630000	0.160490000
0.455510000	0.243910000	0.160870000
0.492330000	0.326220000	0.077300000
0.501970000	0.404190000	0.328450000

0.472740000	0.455790000	0.242260000
0.348420000	0.484030000	0.244080000
0.420750000	0.484580000	0.326740000
0.267640000	0.457660000	0.327490000
0.185100000	0.411070000	0.243860000
0.050500000	0.264100000	0.243630000
0.109320000	0.343930000	0.326990000
0.015750000	0.181610000	0.327050000
0.010980000	0.107630000	0.243770000
0.087590000	0.021340000	0.243800000
0.036320000	0.052050000	0.327130000
0.158540000	0.019770000	0.327110000
0.239690000	0.045880000	0.243770000
0.396520000	0.163920000	0.243980000
0.321900000	0.095370000	0.327180000
0.454280000	0.244110000	0.327410000
0.490830000	0.326670000	0.244320000
0.521450000	0.408410000	0.493950000
0.488250000	0.474120000	0.402340000
0.348670000	0.482030000	0.410890000
0.423760000	0.486660000	0.493590000
0.267600000	0.456690000	0.493690000
0.185030000	0.410480000	0.410450000
0.050180000	0.264060000	0.410350000
0.109140000	0.343880000	0.493720000
0.015670000	0.181600000	0.493750000
0.011020000	0.107680000	0.410430000
0.087650000	0.021390000	0.410460000
0.036400000	0.052130000	0.493780000
0.158540000	0.019720000	0.493810000

0.239610000	0.045580000	0.410470000
0.396280000	0.164000000	0.410610000
0.321880000	0.095230000	0.493830000
0.454680000	0.244330000	0.493830000
0.491920000	0.327090000	0.410340000
0.501860000	0.403890000	0.659350000
0.487560000	0.473140000	0.584910000
0.348660000	0.482010000	0.576450000
0.420610000	0.484320000	0.660610000
0.267630000	0.457680000	0.659890000
0.185030000	0.410490000	0.576960000
0.050170000	0.264070000	0.577120000
0.109300000	0.343940000	0.660450000
0.015740000	0.181620000	0.660450000
0.011020000	0.107700000	0.577090000
0.087680000	0.021430000	0.577130000
0.036360000	0.052100000	0.660420000
0.158590000	0.019880000	0.660510000
0.239630000	0.045640000	0.577180000
0.396350000	0.163980000	0.577060000
0.321950000	0.095410000	0.660490000
0.454520000	0.244040000	0.660300000
0.492050000	0.327000000	0.577390000
0.498120000	0.400570000	0.827270000
0.472690000	0.455620000	0.745250000
0.348400000	0.484010000	0.743290000
0.419780000	0.484590000	0.827310000
0.267550000	0.459630000	0.826720000
0.185080000	0.411090000	0.743550000
0.050470000	0.264110000	0.743840000

0.109610000	0.344060000	0.827100000
0.015880000	0.181630000	0.827120000
0.010990000	0.107650000	0.743750000
0.087640000	0.021430000	0.743790000
0.036240000	0.051990000	0.827090000
0.158640000	0.020070000	0.827170000
0.239730000	0.045990000	0.743880000
0.396650000	0.163870000	0.743720000
0.322070000	0.095660000	0.827190000
0.455730000	0.243840000	0.826900000
0.491100000	0.326590000	0.743460000
0.498090000	0.400420000	0.993830000
0.471760000	0.455220000	0.910960000
0.348670000	0.486150000	0.910210000
0.419900000	0.485360000	0.993670000
0.267560000	0.460450000	0.993690000
0.185090000	0.411630000	0.910320000
0.050790000	0.264150000	0.910450000
0.109760000	0.344100000	0.993720000
0.015960000	0.181640000	0.993750000
0.010950000	0.107600000	0.910430000
0.087580000	0.021380000	0.910450000
0.036170000	0.051920000	0.993780000
0.158640000	0.020110000	0.993800000
0.239790000	0.046280000	0.910520000
0.397090000	0.163850000	0.910450000
0.322130000	0.095820000	0.993840000
0.456460000	0.243620000	0.993890000
0.492440000	0.326200000	0.910470000
0.546620000	0.550660000	0.584110000

0.532260000	0.475130000	0.493810000
0.550500000	0.552440000	0.408260000
0.620910000	0.544830000	0.505570000

(6) Mn_4/BNNT (10, 10) ($G = -272696.0826$ eV)

1.0

31.9069995880	0.0000000000	0.0000000000
-15.9534997940	27.6322722018	0.0000000000
0.0000000000	0.0000000000	14.7571001053

N	B	Mn
120	119	4

Direct

0.513810000	0.449470000	0.015770000
0.477230000	0.491690000	0.099220000
0.420560000	0.511600000	0.016280000
0.271530000	0.480060000	0.016270000
0.349440000	0.506110000	0.099790000
0.192430000	0.434060000	0.099530000
0.119300000	0.371040000	0.016190000
0.020570000	0.216720000	0.016250000
0.059430000	0.296000000	0.099520000
0.005730000	0.141860000	0.099630000
0.015900000	0.078800000	0.016310000
0.106880000	0.014120000	0.016330000
0.050650000	0.034450000	0.099660000
0.177900000	0.019080000	0.099650000
0.256250000	0.047590000	0.016340000
0.407910000	0.159000000	0.016510000
0.334950000	0.095290000	0.099730000
0.468030000	0.233860000	0.100110000
0.510290000	0.312720000	0.016550000

0.526030000	0.387930000	0.099720000
0.514890000	0.449980000	0.181650000
0.478180000	0.491690000	0.265950000
0.419830000	0.509470000	0.183210000
0.271390000	0.479260000	0.183040000
0.349020000	0.504080000	0.266630000
0.192240000	0.433880000	0.266180000
0.119080000	0.371060000	0.182810000
0.020510000	0.216730000	0.182920000
0.059220000	0.296020000	0.266190000
0.005760000	0.141900000	0.266290000
0.015960000	0.078850000	0.182990000
0.106870000	0.014070000	0.182990000
0.050690000	0.034470000	0.266330000
0.177820000	0.018860000	0.266320000
0.256160000	0.047290000	0.183000000
0.407380000	0.159160000	0.183230000
0.334790000	0.095160000	0.266430000
0.466790000	0.234290000	0.266660000
0.508780000	0.313380000	0.183570000
0.530500000	0.391210000	0.267770000
0.532400000	0.466610000	0.341530000
0.481680000	0.493930000	0.432730000
0.419740000	0.507720000	0.350030000
0.271190000	0.478430000	0.349610000
0.348730000	0.503010000	0.432830000
0.192130000	0.433790000	0.432870000
0.118860000	0.371090000	0.349510000
0.020450000	0.216740000	0.349590000
0.059120000	0.296030000	0.432910000

0.005780000	0.141910000	0.432950000
0.016010000	0.078890000	0.349640000
0.106850000	0.014000000	0.349660000
0.050690000	0.034460000	0.432980000
0.177770000	0.018750000	0.433030000
0.256070000	0.047020000	0.349690000
0.407100000	0.159370000	0.349860000
0.334720000	0.095080000	0.433060000
0.467290000	0.234500000	0.433050000
0.510500000	0.313790000	0.349560000
0.548420000	0.392620000	0.433160000
0.531450000	0.465470000	0.523960000
0.477760000	0.491110000	0.599710000
0.419670000	0.507590000	0.515600000
0.271190000	0.478440000	0.516090000
0.349000000	0.504070000	0.599040000
0.192240000	0.433880000	0.599560000
0.118860000	0.371090000	0.516270000
0.020450000	0.216740000	0.516270000
0.059230000	0.296020000	0.599630000
0.005750000	0.141880000	0.599600000
0.015990000	0.078870000	0.516290000
0.106830000	0.013990000	0.516340000
0.050660000	0.034430000	0.599640000
0.177810000	0.018870000	0.599730000
0.256070000	0.047050000	0.516400000
0.407140000	0.159370000	0.516270000
0.334790000	0.095220000	0.599690000
0.467000000	0.234200000	0.599510000
0.510660000	0.313690000	0.516610000

0.530530000	0.390920000	0.598490000
0.514760000	0.449680000	0.684230000
0.476990000	0.491340000	0.766420000
0.419710000	0.509300000	0.682450000
0.271380000	0.479290000	0.682670000
0.349420000	0.506120000	0.765890000
0.192430000	0.434070000	0.766220000
0.119090000	0.371060000	0.682980000
0.020520000	0.216730000	0.682940000
0.059440000	0.295990000	0.766300000
0.005710000	0.141840000	0.766270000
0.015930000	0.078820000	0.682950000
0.106840000	0.014040000	0.683020000
0.050620000	0.034420000	0.766310000
0.177900000	0.019090000	0.766390000
0.256160000	0.047360000	0.683080000
0.407430000	0.159160000	0.682920000
0.334950000	0.095360000	0.766390000
0.468190000	0.233780000	0.766110000
0.509090000	0.313270000	0.682670000
0.526150000	0.387860000	0.766430000
0.513760000	0.449370000	0.850090000
0.477550000	0.492450000	0.932820000
0.420510000	0.511530000	0.849360000
0.271520000	0.480070000	0.849460000
0.349650000	0.506990000	0.932840000
0.192520000	0.434150000	0.932880000
0.119310000	0.371040000	0.849600000
0.020580000	0.216720000	0.849600000
0.059540000	0.295990000	0.932910000

0.005700000	0.141830000	0.932950000
0.015880000	0.078790000	0.849620000
0.106870000	0.014100000	0.849680000
0.050620000	0.034420000	0.932990000
0.177930000	0.019190000	0.933020000
0.256250000	0.047630000	0.849730000
0.407920000	0.159010000	0.849660000
0.335050000	0.095440000	0.933060000
0.469010000	0.233420000	0.933120000
0.510390000	0.312690000	0.849700000
0.526130000	0.387740000	0.933060000
0.491080000	0.479020000	0.015820000
0.519530000	0.429560000	0.098760000
0.440510000	0.505780000	0.099440000
0.374180000	0.509860000	0.016280000
0.219020000	0.450730000	0.016240000
0.298010000	0.489910000	0.099690000
0.143280000	0.393280000	0.099530000
0.078600000	0.321880000	0.016220000
0.009130000	0.166560000	0.016280000
0.032140000	0.243430000	0.099560000
0.010980000	0.099160000	0.099640000
0.037470000	0.048040000	0.016320000
0.153240000	0.015820000	0.016340000
0.086730000	0.019340000	0.099670000
0.229590000	0.036510000	0.099650000
0.308620000	0.078200000	0.016350000
0.449140000	0.207930000	0.016650000
0.383760000	0.136710000	0.099800000
0.496890000	0.286380000	0.100400000

0.522430000	0.362980000	0.016580000
0.491570000	0.478890000	0.182030000
0.527130000	0.435260000	0.265380000
0.440230000	0.504020000	0.266190000
0.373670000	0.508030000	0.183120000
0.218880000	0.450390000	0.182950000
0.297790000	0.488650000	0.266420000
0.143040000	0.393250000	0.266190000
0.078400000	0.321900000	0.182850000
0.009130000	0.166590000	0.182940000
0.032020000	0.243450000	0.266230000
0.011030000	0.099210000	0.266310000
0.037520000	0.048080000	0.183000000
0.153200000	0.015690000	0.182990000
0.086730000	0.019300000	0.266330000
0.229500000	0.036240000	0.266330000
0.308510000	0.078010000	0.183030000
0.448090000	0.208320000	0.183440000
0.383430000	0.136820000	0.266540000
0.496110000	0.286750000	0.267020000
0.522840000	0.364290000	0.184530000
0.498050000	0.484150000	0.348070000
0.441340000	0.503750000	0.432790000
0.373420000	0.506220000	0.349800000
0.218700000	0.450050000	0.349570000
0.297620000	0.488000000	0.432850000
0.142910000	0.393240000	0.432890000
0.078200000	0.321910000	0.349550000
0.009130000	0.166610000	0.349610000
0.031970000	0.243450000	0.432930000

0.011050000	0.099230000	0.432960000
0.037540000	0.048090000	0.349660000
0.153150000	0.015550000	0.349670000
0.086710000	0.019270000	0.433000000
0.229450000	0.036110000	0.433040000
0.308400000	0.077830000	0.349720000
0.447770000	0.208620000	0.350020000
0.383320000	0.136830000	0.433070000
0.497630000	0.287120000	0.433050000
0.531390000	0.366520000	0.350940000
0.497520000	0.483590000	0.517330000
0.526830000	0.434700000	0.600730000
0.440030000	0.503750000	0.599470000
0.373390000	0.506180000	0.515860000
0.218700000	0.450060000	0.516160000
0.297780000	0.488670000	0.599280000
0.143040000	0.393250000	0.599580000
0.078200000	0.321910000	0.516270000
0.009130000	0.166610000	0.516280000
0.032030000	0.243440000	0.599620000
0.011010000	0.099190000	0.599620000
0.037530000	0.048070000	0.516310000
0.153140000	0.015540000	0.516370000
0.086700000	0.019270000	0.599660000
0.229500000	0.036270000	0.599750000
0.308400000	0.077860000	0.516400000
0.447860000	0.208590000	0.516110000
0.383460000	0.136850000	0.599600000
0.496350000	0.286650000	0.599190000
0.531540000	0.366380000	0.515250000

0.491200000	0.478390000	0.683660000
0.519530000	0.429400000	0.767260000
0.440370000	0.505560000	0.766220000
0.373620000	0.507990000	0.682560000
0.218880000	0.450410000	0.682790000
0.298000000	0.489940000	0.766020000
0.143290000	0.393280000	0.766250000
0.078410000	0.321890000	0.682960000
0.009130000	0.166580000	0.682950000
0.032150000	0.243430000	0.766290000
0.010960000	0.099150000	0.766280000
0.037480000	0.048040000	0.682970000
0.153190000	0.015680000	0.683050000
0.086700000	0.019300000	0.766330000
0.229590000	0.036550000	0.766420000
0.308520000	0.078070000	0.683080000
0.448230000	0.208260000	0.682750000
0.383780000	0.136730000	0.766350000
0.497090000	0.286290000	0.765870000
0.523010000	0.364130000	0.681740000
0.490980000	0.478860000	0.849900000
0.519580000	0.429520000	0.933000000
0.440940000	0.506790000	0.932820000
0.374160000	0.509850000	0.849390000
0.219010000	0.450740000	0.849510000
0.298120000	0.490500000	0.932860000
0.143400000	0.393290000	0.932890000
0.078600000	0.321880000	0.849600000
0.009130000	0.166550000	0.849610000
0.032200000	0.243430000	0.932920000

0.010940000	0.099130000	0.932960000
0.037450000	0.048020000	0.849640000
0.153240000	0.015810000	0.849700000
0.086710000	0.019340000	0.933000000
0.229630000	0.036670000	0.933030000
0.308620000	0.078230000	0.849750000
0.449200000	0.207910000	0.849580000
0.383990000	0.136690000	0.933080000
0.497950000	0.285910000	0.933140000
0.522510000	0.362940000	0.849630000
0.658720000	0.517890000	0.449200000
0.594780000	0.535670000	0.523470000
0.599630000	0.536480000	0.347470000
0.570440000	0.459920000	0.433300000

(7) Mn_4/h-BN (0001) ($G = -66769.2425$ eV)

1.0

12.5621004105	0.0000000000	0.0000000000
-6.2810502052	10.8790980804	0.0000000000
0.0000000000	0.0000000000	22.7073001862

B   N   Mn

24   25   4

Direct

0.106420000	0.034480000	0.079840000
0.306490000	0.034400000	0.080660000
0.506690000	0.034630000	0.079950000
0.706680000	0.034880000	0.080580000
0.906640000	0.034780000	0.080400000
0.107270000	0.234910000	0.085250000
0.305020000	0.231290000	0.096900000
0.505110000	0.231430000	0.096650000

0.706140000	0.234960000	0.085370000
0.906510000	0.234680000	0.080480000
0.105910000	0.434400000	0.080150000
0.303450000	0.435110000	0.097740000
0.709720000	0.435950000	0.095390000
0.906730000	0.434550000	0.079530000
0.106460000	0.634630000	0.075010000
0.306220000	0.635060000	0.081160000
0.506310000	0.637980000	0.097170000
0.709810000	0.636280000	0.095240000
0.906830000	0.634760000	0.079890000
0.106580000	0.834770000	0.074880000
0.306740000	0.834930000	0.075190000
0.506890000	0.835490000	0.080020000
0.706370000	0.834190000	0.084680000
0.906880000	0.835030000	0.079380000
0.040090000	0.101540000	0.081560000
0.238900000	0.100190000	0.083690000
0.439780000	0.100150000	0.083590000
0.639960000	0.101410000	0.081750000
0.839960000	0.101370000	0.080470000
0.040100000	0.301250000	0.081580000
0.239840000	0.301330000	0.094540000
0.432290000	0.286320000	0.111720000
0.640070000	0.301070000	0.094420000
0.839730000	0.301210000	0.081370000
0.039980000	0.501220000	0.076310000
0.238870000	0.501510000	0.084620000
0.431580000	0.510240000	0.116050000
0.653870000	0.508460000	0.108800000

0.841130000	0.501420000	0.082800000
0.039970000	0.701350000	0.074780000
0.240010000	0.701360000	0.075430000
0.439760000	0.702470000	0.084270000
0.639930000	0.701560000	0.093410000
0.841100000	0.702460000	0.082650000
0.039930000	0.901440000	0.076280000
0.239940000	0.901300000	0.075120000
0.440050000	0.901400000	0.076610000
0.640010000	0.901300000	0.081380000
0.839740000	0.901300000	0.081040000
0.606010000	0.549590000	0.249700000
0.511400000	0.432670000	0.153520000
0.387570000	0.334220000	0.248140000
0.408620000	0.534420000	0.204640000

(8)   Fe$_4$/BNNT (6, 6) ($G = -170974.8378$ eV)

  1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

  B   N   Fe

 71   72   4

Direct

0.395060000	0.331900000	0.008720000
0.354410000	0.385220000	0.092340000
0.276900000	0.393600000	0.009970000
0.097390000	0.278120000	0.010380000
0.183510000	0.354300000	0.093790000
0.042610000	0.184040000	0.093560000
0.034640000	0.098850000	0.010130000

0.153820000	0.039110000	0.010300000
0.075460000	0.045730000	0.093480000
0.247650000	0.079570000	0.093970000
0.334220000	0.155400000	0.010930000
0.389900000	0.249700000	0.095460000
0.401730000	0.337680000	0.175280000
0.361390000	0.392490000	0.257840000
0.277830000	0.392980000	0.176590000
0.097800000	0.277600000	0.177120000
0.184570000	0.353050000	0.260530000
0.042280000	0.183640000	0.260200000
0.034080000	0.098390000	0.176780000
0.153570000	0.039280000	0.177070000
0.075020000	0.045440000	0.260220000
0.247650000	0.080420000	0.260660000
0.333670000	0.156330000	0.177520000
0.402790000	0.248750000	0.260930000
0.361150000	0.391940000	0.428960000
0.279790000	0.392550000	0.343500000
0.097880000	0.277200000	0.343510000
0.184530000	0.352980000	0.426480000
0.042240000	0.183650000	0.426880000
0.033770000	0.098160000	0.343580000
0.153440000	0.039410000	0.343630000
0.075060000	0.045480000	0.427000000
0.247700000	0.080360000	0.426610000
0.335640000	0.156140000	0.343630000
0.402940000	0.248530000	0.426390000
0.401610000	0.337090000	0.511810000
0.354320000	0.384790000	0.594570000

0.277750000	0.392620000	0.510380000
0.097720000	0.277590000	0.509930000
0.183480000	0.354190000	0.593200000
0.042540000	0.184030000	0.593540000
0.034080000	0.098410000	0.510360000
0.153630000	0.039330000	0.510180000
0.075530000	0.045810000	0.593720000
0.247730000	0.079470000	0.593330000
0.333860000	0.156110000	0.509820000
0.390100000	0.249470000	0.591930000
0.395110000	0.331750000	0.678430000
0.353750000	0.384690000	0.760600000
0.276880000	0.393370000	0.676950000
0.097330000	0.278110000	0.676670000
0.182940000	0.355030000	0.760030000
0.042780000	0.184330000	0.760220000
0.034640000	0.098870000	0.677010000
0.153880000	0.039160000	0.676950000
0.075950000	0.046130000	0.760330000
0.248150000	0.078680000	0.760150000
0.334350000	0.155230000	0.676460000
0.389810000	0.248020000	0.760110000
0.395680000	0.332230000	0.843580000
0.353760000	0.384810000	0.926340000
0.276690000	0.393770000	0.843460000
0.097220000	0.278310000	0.843530000
0.182940000	0.355090000	0.926940000
0.042810000	0.184340000	0.926890000
0.034900000	0.099080000	0.843570000
0.154090000	0.039200000	0.843620000

0.075920000	0.046100000	0.926850000
0.248120000	0.078720000	0.927180000
0.334730000	0.154380000	0.843700000
0.389780000	0.248110000	0.927250000
0.387970000	0.355560000	0.091070000
0.332590000	0.395410000	0.009450000
0.151190000	0.334080000	0.010490000
0.246770000	0.387530000	0.093720000
0.072680000	0.247390000	0.093650000
0.031800000	0.152260000	0.010120000
0.097320000	0.035730000	0.010210000
0.040550000	0.074100000	0.093410000
0.184360000	0.045490000	0.093810000
0.279880000	0.099910000	0.010750000
0.400550000	0.280230000	0.010490000
0.358900000	0.186380000	0.094220000
0.405010000	0.374990000	0.249460000
0.334480000	0.397270000	0.175810000
0.152080000	0.333050000	0.177350000
0.247950000	0.385810000	0.260750000
0.072690000	0.246960000	0.260220000
0.031310000	0.151840000	0.176760000
0.096850000	0.035440000	0.176930000
0.039990000	0.073690000	0.260170000
0.184340000	0.046080000	0.260470000
0.279300000	0.101160000	0.177290000
0.404450000	0.282860000	0.179820000
0.360850000	0.186050000	0.259990000
0.404350000	0.373890000	0.437350000
0.338210000	0.399210000	0.343490000

0.152420000	0.332270000	0.343500000
0.247900000	0.385590000	0.426250000
0.072630000	0.246970000	0.426810000
0.031020000	0.151620000	0.343550000
0.096620000	0.035310000	0.343620000
0.040010000	0.073720000	0.427010000
0.184370000	0.046090000	0.426780000
0.279850000	0.101710000	0.343620000
0.435140000	0.275440000	0.343690000
0.361040000	0.185840000	0.427320000
0.388020000	0.355290000	0.595980000
0.334250000	0.396630000	0.511090000
0.152010000	0.333020000	0.509660000
0.246730000	0.387270000	0.593240000
0.072590000	0.247390000	0.593410000
0.031280000	0.151850000	0.510350000
0.096930000	0.035520000	0.510290000
0.040590000	0.074150000	0.593750000
0.184420000	0.045520000	0.593450000
0.279390000	0.101000000	0.510000000
0.404600000	0.282510000	0.507580000
0.359110000	0.186120000	0.593150000
0.388480000	0.356200000	0.760980000
0.332560000	0.395180000	0.677430000
0.151150000	0.334030000	0.676520000
0.246290000	0.388190000	0.760070000
0.072500000	0.247690000	0.760150000
0.031760000	0.152260000	0.676990000
0.097390000	0.035810000	0.676990000
0.041090000	0.074550000	0.760320000

0.184740000	0.045370000	0.760210000
0.279950000	0.099770000	0.676600000
0.400590000	0.280060000	0.676820000
0.359890000	0.184720000	0.760220000
0.388440000	0.356260000	0.926080000
0.332390000	0.395470000	0.843450000
0.150910000	0.334390000	0.843500000
0.246300000	0.388290000	0.926840000
0.072540000	0.247690000	0.926930000
0.031980000	0.152440000	0.843560000
0.097660000	0.036000000	0.843590000
0.041070000	0.074520000	0.926820000
0.184710000	0.045360000	0.927060000
0.280180000	0.099060000	0.843680000
0.400480000	0.279890000	0.843640000
0.359820000	0.184810000	0.927180000
0.499890000	0.423810000	0.266470000
0.499120000	0.421860000	0.423660000
0.429400000	0.345210000	0.342980000
0.519580000	0.355690000	0.343150000

(9)　　Nb$_4$/BNNT (6, 6) ($G = -164393.8584$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B　　N　　Nb

71　　72　　4

Direct

0.393930000	0.331420000	0.011180000
0.354800000	0.385760000	0.094410000

0.277150000	0.393550000	0.011690000
0.097350000	0.278960000	0.012060000
0.183710000	0.354570000	0.095480000
0.042830000	0.184940000	0.095190000
0.035080000	0.099770000	0.011810000
0.153570000	0.038860000	0.011850000
0.075840000	0.046580000	0.095180000
0.247230000	0.077390000	0.095510000
0.333310000	0.153570000	0.012520000
0.385880000	0.247700000	0.097050000
0.401110000	0.337650000	0.179530000
0.362120000	0.391570000	0.261170000
0.278040000	0.392340000	0.178770000
0.097500000	0.278580000	0.178600000
0.184020000	0.354060000	0.261860000
0.042600000	0.184780000	0.261820000
0.034710000	0.099490000	0.178480000
0.153420000	0.038950000	0.178810000
0.075580000	0.046510000	0.261950000
0.247480000	0.078360000	0.262440000
0.332740000	0.154010000	0.179000000
0.397160000	0.247530000	0.261870000
0.354100000	0.384170000	0.429890000
0.278640000	0.392450000	0.344740000
0.097340000	0.278600000	0.344990000
0.183540000	0.354730000	0.427880000
0.042680000	0.184980000	0.428500000
0.034520000	0.099470000	0.345240000
0.153590000	0.039650000	0.345490000
0.075650000	0.046750000	0.428690000

0.247960000	0.079490000	0.428530000
0.335540000	0.154190000	0.345050000
0.401610000	0.247570000	0.426600000
0.394010000	0.329910000	0.512650000
0.350330000	0.380630000	0.595540000
0.275970000	0.392540000	0.511980000
0.097150000	0.279110000	0.511560000
0.182440000	0.355830000	0.594980000
0.042930000	0.185340000	0.595180000
0.034750000	0.099750000	0.511980000
0.154000000	0.040260000	0.511950000
0.076010000	0.047070000	0.595330000
0.248180000	0.079340000	0.595000000
0.335280000	0.154810000	0.511350000
0.391940000	0.247820000	0.594240000
0.393090000	0.329100000	0.679600000
0.352350000	0.383020000	0.761650000
0.275820000	0.393160000	0.678510000
0.096840000	0.279400000	0.678480000
0.182430000	0.356020000	0.761920000
0.043050000	0.185420000	0.761910000
0.035120000	0.100050000	0.678620000
0.154170000	0.040080000	0.678480000
0.076250000	0.047170000	0.761890000
0.248200000	0.078130000	0.761690000
0.335300000	0.153890000	0.678380000
0.389870000	0.246820000	0.762310000
0.394660000	0.331150000	0.845260000
0.353760000	0.384840000	0.927850000
0.276440000	0.393620000	0.845030000

0.097000000	0.279300000	0.845350000
0.182990000	0.355580000	0.928750000
0.043020000	0.185240000	0.928580000
0.035270000	0.100040000	0.845210000
0.154020000	0.039490000	0.845080000
0.076150000	0.046910000	0.928460000
0.247770000	0.077320000	0.928620000
0.334610000	0.153100000	0.845580000
0.388100000	0.246840000	0.929370000
0.388080000	0.356050000	0.093730000
0.333190000	0.396150000	0.011190000
0.151280000	0.334690000	0.012230000
0.247010000	0.386810000	0.095600000
0.072500000	0.248210000	0.095230000
0.032210000	0.153150000	0.011790000
0.097510000	0.036410000	0.011820000
0.041080000	0.075080000	0.095130000
0.183910000	0.044510000	0.095390000
0.279520000	0.097670000	0.012270000
0.397550000	0.278660000	0.012580000
0.357190000	0.184560000	0.095860000
0.408820000	0.376440000	0.255620000
0.334870000	0.396560000	0.178750000
0.151750000	0.333930000	0.178680000
0.247350000	0.385940000	0.261890000
0.072360000	0.248030000	0.261780000
0.031870000	0.152880000	0.178450000
0.097240000	0.036240000	0.178650000
0.040710000	0.074880000	0.261890000
0.184120000	0.045320000	0.262260000

0.279090000	0.098270000	0.178890000
0.397540000	0.279780000	0.181410000
0.359610000	0.184190000	0.261380000
0.389770000	0.358230000	0.433810000
0.335970000	0.396960000	0.344590000
0.151520000	0.333980000	0.344780000
0.246820000	0.386750000	0.427470000
0.072350000	0.248250000	0.428400000
0.031750000	0.152900000	0.345220000
0.097180000	0.036410000	0.345390000
0.040680000	0.075000000	0.428660000
0.184600000	0.046400000	0.428640000
0.280010000	0.099590000	0.345330000
0.429260000	0.277890000	0.342490000
0.362100000	0.184420000	0.428130000
0.382500000	0.349620000	0.596780000
0.330520000	0.392960000	0.512570000
0.150950000	0.334960000	0.511260000
0.245640000	0.388280000	0.595110000
0.072320000	0.248640000	0.595090000
0.032040000	0.153220000	0.511970000
0.097520000	0.036830000	0.511980000
0.041050000	0.075340000	0.595340000
0.184840000	0.046480000	0.595120000
0.280060000	0.100300000	0.511660000
0.405270000	0.280350000	0.509520000
0.361000000	0.184420000	0.594980000
0.386940000	0.354280000	0.762010000
0.330520000	0.393030000	0.678740000
0.150290000	0.335560000	0.678470000

0.245760000	0.388390000	0.761990000
0.072280000	0.248700000	0.761910000
0.032350000	0.153480000	0.678590000
0.097840000	0.037020000	0.678550000
0.041400000	0.075530000	0.761900000
0.184810000	0.045820000	0.761720000
0.280350000	0.098980000	0.678330000
0.401050000	0.278680000	0.678710000
0.360380000	0.183490000	0.762320000
0.388070000	0.355870000	0.927810000
0.331910000	0.394830000	0.844760000
0.150620000	0.335340000	0.845480000
0.246340000	0.388250000	0.928690000
0.072440000	0.248520000	0.928640000
0.032410000	0.153430000	0.845190000
0.097880000	0.036860000	0.845130000
0.041400000	0.075390000	0.928460000
0.184380000	0.044940000	0.928530000
0.280110000	0.097770000	0.845330000
0.399320000	0.278660000	0.845720000
0.358990000	0.183570000	0.929190000
0.505320000	0.408470000	0.199340000
0.573740000	0.426900000	0.335050000
0.457930000	0.366900000	0.359750000
0.522470000	0.330300000	0.257610000

(10) $^{*}N_2$ adsorption on Mn_4/BNNT (6, 6) ($G = -171621.8246$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B   N   Mn

71   74   4

Direct

0.401140000	0.329800000	0.010920000
0.361450000	0.383080000	0.094480000
0.284220000	0.392370000	0.011980000
0.102840000	0.283810000	0.012370000
0.190880000	0.356570000	0.095700000
0.043980000	0.190520000	0.095780000
0.031400000	0.103430000	0.012560000
0.146160000	0.039000000	0.012930000
0.069080000	0.047660000	0.096060000
0.239660000	0.077510000	0.096750000
0.327730000	0.151210000	0.013850000
0.390030000	0.244770000	0.096780000
0.416580000	0.341760000	0.177320000
0.366530000	0.388890000	0.261150000
0.284540000	0.391060000	0.178680000
0.102810000	0.283450000	0.179090000
0.191320000	0.355710000	0.262350000
0.043700000	0.190290000	0.262450000
0.031090000	0.103180000	0.179270000
0.145780000	0.038800000	0.179730000
0.068890000	0.047500000	0.262900000
0.239560000	0.077540000	0.263350000
0.326480000	0.152710000	0.180590000
0.395810000	0.244060000	0.266030000
0.364440000	0.383700000	0.429090000
0.285370000	0.390190000	0.345360000
0.102750000	0.283240000	0.345600000

0.191290000	0.355570000	0.428530000
0.043700000	0.190340000	0.429150000
0.031030000	0.103140000	0.346040000
0.145840000	0.038750000	0.346450000
0.069210000	0.047770000	0.429660000
0.239970000	0.076590000	0.429590000
0.327970000	0.151250000	0.346640000
0.395710000	0.242370000	0.429880000
0.403990000	0.330340000	0.512860000
0.360800000	0.381800000	0.595650000
0.284550000	0.390460000	0.511740000
0.102830000	0.283490000	0.512150000
0.191040000	0.356600000	0.595140000
0.043980000	0.190590000	0.595820000
0.031300000	0.103360000	0.512760000
0.146320000	0.038980000	0.513050000
0.069720000	0.048190000	0.596280000
0.240320000	0.075880000	0.596340000
0.328300000	0.149610000	0.512850000
0.388810000	0.242130000	0.595880000
0.399630000	0.327730000	0.679710000
0.360730000	0.382950000	0.761990000
0.284450000	0.392420000	0.678450000
0.102890000	0.283870000	0.678840000
0.190850000	0.357440000	0.761940000
0.044220000	0.190780000	0.762460000
0.031610000	0.103610000	0.679370000
0.146680000	0.039220000	0.679720000
0.069900000	0.048360000	0.762820000
0.240590000	0.075790000	0.763210000

0.328870000	0.148860000	0.679660000
0.388470000	0.241560000	0.762930000
0.399810000	0.328340000	0.845210000
0.360560000	0.383040000	0.928140000
0.284380000	0.393200000	0.845190000
0.102900000	0.284000000	0.845600000
0.190770000	0.357430000	0.928850000
0.044210000	0.190740000	0.929110000
0.031650000	0.103640000	0.845940000
0.146660000	0.039270000	0.846310000
0.069590000	0.048100000	0.929350000
0.240310000	0.076480000	0.930100000
0.328900000	0.149120000	0.846870000
0.389130000	0.242660000	0.929590000
0.396900000	0.355620000	0.093260000
0.339500000	0.393410000	0.011660000
0.158610000	0.337790000	0.012310000
0.254120000	0.386630000	0.095670000
0.076770000	0.253870000	0.095660000
0.031750000	0.158470000	0.012410000
0.090290000	0.036890000	0.012760000
0.035920000	0.077820000	0.095900000
0.176410000	0.044630000	0.096460000
0.272120000	0.097250000	0.013720000
0.403490000	0.276030000	0.012510000
0.353030000	0.182150000	0.097160000
0.413900000	0.375740000	0.255650000
0.340650000	0.393800000	0.178300000
0.158870000	0.337060000	0.179120000
0.254630000	0.385270000	0.262370000

0.076550000	0.253620000	0.262300000
0.031430000	0.158220000	0.179080000
0.089820000	0.036500000	0.179510000
0.035710000	0.077670000	0.262690000
0.176270000	0.044550000	0.263070000
0.271430000	0.098390000	0.180030000
0.409960000	0.278930000	0.180860000
0.353040000	0.182010000	0.263350000
0.403910000	0.361150000	0.433000000
0.342100000	0.393570000	0.345210000
0.158950000	0.336610000	0.345440000
0.254480000	0.384840000	0.428200000
0.076560000	0.253660000	0.428970000
0.031250000	0.158120000	0.345850000
0.089910000	0.036570000	0.346290000
0.035900000	0.077810000	0.429470000
0.176550000	0.044460000	0.429590000
0.271890000	0.097360000	0.346280000
0.421150000	0.273060000	0.348020000
0.355010000	0.179350000	0.430080000
0.394410000	0.352390000	0.596770000
0.339820000	0.391740000	0.511710000
0.158900000	0.337040000	0.511850000
0.254290000	0.386660000	0.594860000
0.076770000	0.253930000	0.595640000
0.031440000	0.158290000	0.512590000
0.090500000	0.037070000	0.512970000
0.036300000	0.078110000	0.596130000
0.176930000	0.044530000	0.596340000
0.272180000	0.095940000	0.512870000

0.403820000	0.274950000	0.512890000
0.354870000	0.178680000	0.596380000
0.394250000	0.353190000	0.762430000
0.339730000	0.393410000	0.678570000
0.158710000	0.337800000	0.678580000
0.254200000	0.388070000	0.761760000
0.076940000	0.254130000	0.762300000
0.031760000	0.158540000	0.679230000
0.090940000	0.037450000	0.679590000
0.036480000	0.078250000	0.762690000
0.177190000	0.044740000	0.763100000
0.272670000	0.095190000	0.679760000
0.400860000	0.273620000	0.679890000
0.355340000	0.178200000	0.763350000
0.394220000	0.353480000	0.927910000
0.339750000	0.394230000	0.845090000
0.158600000	0.338100000	0.845430000
0.254120000	0.388070000	0.928720000
0.076920000	0.254100000	0.928970000
0.031890000	0.158620000	0.845810000
0.090890000	0.037410000	0.846150000
0.036290000	0.078120000	0.929240000
0.176950000	0.044770000	0.929840000
0.272700000	0.095560000	0.846880000
0.401200000	0.274170000	0.845980000
0.354990000	0.179410000	0.930330000
0.561780000	0.421530000	0.195140000
0.582000000	0.387060000	0.212900000
0.496100000	0.425230000	0.221280000
0.556560000	0.395080000	0.335250000

0.451550000	0.355810000	0.348070000
0.499400000	0.333970000	0.185370000

(11)   *NNH adsorption on Mn$_4$/BNNT (6, 6) ($G = -171637.4698$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B   N   Mn   H

71   74   4   1

Direct

0.402670000	0.328430000	0.010340000
0.364070000	0.382510000	0.094080000
0.286940000	0.392210000	0.011630000
0.105020000	0.285470000	0.011910000
0.193640000	0.357260000	0.095260000
0.044760000	0.192490000	0.095290000
0.030430000	0.104760000	0.012040000
0.143110000	0.038000000	0.012280000
0.066740000	0.047780000	0.095490000
0.236470000	0.075480000	0.096030000
0.324960000	0.148780000	0.013200000
0.388230000	0.242150000	0.096240000
0.417280000	0.339360000	0.176910000
0.368320000	0.387290000	0.260970000
0.287100000	0.390690000	0.178280000
0.104980000	0.285130000	0.178620000
0.194020000	0.356450000	0.261910000
0.044500000	0.192290000	0.261970000
0.030180000	0.104530000	0.178750000
0.142700000	0.037680000	0.179110000

0.066560000	0.047630000	0.262330000
0.236380000	0.075470000	0.262740000
0.323500000	0.150110000	0.179800000
0.392850000	0.241110000	0.265070000
0.366770000	0.383180000	0.428870000
0.287910000	0.390080000	0.344970000
0.104920000	0.284970000	0.345140000
0.194000000	0.356440000	0.428110000
0.044510000	0.192350000	0.428650000
0.030110000	0.104500000	0.345500000
0.142780000	0.037690000	0.345880000
0.066840000	0.047900000	0.429100000
0.236800000	0.074820000	0.429040000
0.325000000	0.148790000	0.346040000
0.394090000	0.239920000	0.428930000
0.405120000	0.329010000	0.512370000
0.362950000	0.381270000	0.595270000
0.287150000	0.390610000	0.511360000
0.105030000	0.285220000	0.511710000
0.193770000	0.357490000	0.594740000
0.044770000	0.192590000	0.595320000
0.030310000	0.104700000	0.512210000
0.143290000	0.038090000	0.512500000
0.067320000	0.048330000	0.595720000
0.237230000	0.074420000	0.595710000
0.325580000	0.147520000	0.512120000
0.387660000	0.239770000	0.595070000
0.400430000	0.326000000	0.679220000
0.362930000	0.382350000	0.761560000
0.287090000	0.392570000	0.678070000

0.105100000	0.285570000	0.678400000
0.193610000	0.358250000	0.761570000
0.044980000	0.192750000	0.761970000
0.030570000	0.104920000	0.678830000
0.143700000	0.038430000	0.679120000
0.067500000	0.048500000	0.762250000
0.237510000	0.074290000	0.762530000
0.326240000	0.146720000	0.678940000
0.387230000	0.239030000	0.762310000
0.400730000	0.326640000	0.844680000
0.363030000	0.382530000	0.927710000
0.287070000	0.393210000	0.844840000
0.105100000	0.285670000	0.845160000
0.193560000	0.358150000	0.928460000
0.044970000	0.192700000	0.928630000
0.030610000	0.104950000	0.845420000
0.143670000	0.038430000	0.845670000
0.067210000	0.048230000	0.928780000
0.237190000	0.074770000	0.929390000
0.326220000	0.146840000	0.846210000
0.387660000	0.240060000	0.929110000
0.399770000	0.355220000	0.092580000
0.342110000	0.392990000	0.011340000
0.161330000	0.338840000	0.011890000
0.256850000	0.386620000	0.095250000
0.078580000	0.255800000	0.095200000
0.031950000	0.160360000	0.011920000
0.087570000	0.036590000	0.012160000
0.034410000	0.078820000	0.095380000
0.173200000	0.043160000	0.095800000

0.269000000	0.095140000	0.013040000
0.402490000	0.273420000	0.012000000
0.350340000	0.179550000	0.096530000
0.414930000	0.373050000	0.255380000
0.342870000	0.392720000	0.177940000
0.161560000	0.338130000	0.178660000
0.257290000	0.385310000	0.261930000
0.078380000	0.255580000	0.261850000
0.031690000	0.160130000	0.178590000
0.087100000	0.036150000	0.178930000
0.034220000	0.078670000	0.262150000
0.173040000	0.043050000	0.262480000
0.268240000	0.095990000	0.179350000
0.407540000	0.275930000	0.180410000
0.349980000	0.179220000	0.262650000
0.406060000	0.360550000	0.432900000
0.344370000	0.392900000	0.344880000
0.161610000	0.337750000	0.344990000
0.257150000	0.385180000	0.427790000
0.078410000	0.255630000	0.428510000
0.031540000	0.160060000	0.345350000
0.087170000	0.036230000	0.345730000
0.034350000	0.078790000	0.428930000
0.173380000	0.043180000	0.429050000
0.268710000	0.095130000	0.345710000
0.419230000	0.270210000	0.346570000
0.352400000	0.177030000	0.429270000
0.395870000	0.351140000	0.596430000
0.342200000	0.391520000	0.511390000
0.161570000	0.338210000	0.511430000

0.256980000	0.387050000	0.594500000
0.078630000	0.255890000	0.595180000
0.031680000	0.160220000	0.512090000
0.087760000	0.036780000	0.512420000
0.034670000	0.079050000	0.595590000
0.173840000	0.043480000	0.595750000
0.269080000	0.094220000	0.512240000
0.403360000	0.272710000	0.512070000
0.352480000	0.176370000	0.595610000
0.395750000	0.351870000	0.761930000
0.342180000	0.393220000	0.678220000
0.161410000	0.338930000	0.678190000
0.256930000	0.388350000	0.761440000
0.078770000	0.256070000	0.761850000
0.031930000	0.160440000	0.678730000
0.088230000	0.037220000	0.679020000
0.034840000	0.079190000	0.762160000
0.174120000	0.043690000	0.762460000
0.269620000	0.093510000	0.679080000
0.400300000	0.271210000	0.679250000
0.352980000	0.175710000	0.762690000
0.396240000	0.352500000	0.927320000
0.342290000	0.393950000	0.844740000
0.161330000	0.339170000	0.845040000
0.256880000	0.388130000	0.928390000
0.078730000	0.256020000	0.928510000
0.032050000	0.160500000	0.845320000
0.088190000	0.037170000	0.845560000
0.034710000	0.079080000	0.928710000
0.173830000	0.043560000	0.929170000

0.269630000	0.093700000	0.846190000
0.400460000	0.271650000	0.845440000
0.352490000	0.176850000	0.929730000
0.577070000	0.443820000	0.211760000
0.574120000	0.389300000	0.211370000
0.496870000	0.426420000	0.221960000
0.559150000	0.399440000	0.336290000
0.453530000	0.353730000	0.348500000
0.497240000	0.326610000	0.202790000
0.618550000	0.477680000	0.200660000

(12)   *HNNH adsorption on Mn$_4$/BNNT (6, 6) ($G = -171653.3507$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B   N   Mn   H

71   74   4   2

Direct

0.401860000	0.327530000	0.010480000
0.363620000	0.381910000	0.094290000
0.287050000	0.392470000	0.011840000
0.105260000	0.285920000	0.012050000
0.193870000	0.357670000	0.095480000
0.044980000	0.192910000	0.095370000
0.030590000	0.105160000	0.012060000
0.143000000	0.038030000	0.012220000
0.066750000	0.048050000	0.095470000
0.236340000	0.075160000	0.095930000
0.324980000	0.148200000	0.013040000
0.388360000	0.241520000	0.095950000

0.416600000	0.338420000	0.177040000
0.368450000	0.387040000	0.261200000
0.287350000	0.390910000	0.178530000
0.105220000	0.285530000	0.178760000
0.194290000	0.356760000	0.262100000
0.044700000	0.192690000	0.262040000
0.030300000	0.104910000	0.178770000
0.142570000	0.037700000	0.179040000
0.066530000	0.047860000	0.262290000
0.236190000	0.075210000	0.262650000
0.323520000	0.149590000	0.179680000
0.392470000	0.240730000	0.264990000
0.367120000	0.383450000	0.429140000
0.288200000	0.390220000	0.345160000
0.105160000	0.285350000	0.345270000
0.194280000	0.356750000	0.428250000
0.044720000	0.192750000	0.428730000
0.030220000	0.104870000	0.345530000
0.142580000	0.037640000	0.345800000
0.066770000	0.048090000	0.429070000
0.236520000	0.074630000	0.428960000
0.324700000	0.148590000	0.346000000
0.393480000	0.240030000	0.428780000
0.405220000	0.329300000	0.512600000
0.363080000	0.381470000	0.595570000
0.287420000	0.390870000	0.511550000
0.105280000	0.285630000	0.511810000
0.194020000	0.357900000	0.594880000
0.045020000	0.193020000	0.595400000
0.030450000	0.105070000	0.512250000

0.143040000	0.037990000	0.512430000
0.067250000	0.048520000	0.595710000
0.236960000	0.074210000	0.595580000
0.325220000	0.147460000	0.511980000
0.387280000	0.239680000	0.594930000
0.400180000	0.325830000	0.679420000
0.362860000	0.382300000	0.761830000
0.287290000	0.392940000	0.678290000
0.105350000	0.286020000	0.678500000
0.193810000	0.358740000	0.761710000
0.045250000	0.193200000	0.762050000
0.030740000	0.105320000	0.678870000
0.143480000	0.038350000	0.679060000
0.067490000	0.048730000	0.762240000
0.237290000	0.074010000	0.762390000
0.325990000	0.146490000	0.678730000
0.386940000	0.238710000	0.762160000
0.400260000	0.326140000	0.844830000
0.362720000	0.382180000	0.927960000
0.287200000	0.393540000	0.845060000
0.105340000	0.286140000	0.845280000
0.193740000	0.358640000	0.928640000
0.045220000	0.193150000	0.928700000
0.030800000	0.105360000	0.845450000
0.143520000	0.038400000	0.845620000
0.067230000	0.048500000	0.928770000
0.237030000	0.074450000	0.929270000
0.326090000	0.146400000	0.845990000
0.387440000	0.239520000	0.928920000
0.398530000	0.353890000	0.092770000

0.341990000	0.392850000	0.011540000
0.161530000	0.339310000	0.012080000
0.257060000	0.387000000	0.095520000
0.078810000	0.256220000	0.095310000
0.032180000	0.160790000	0.011980000
0.087520000	0.036780000	0.012140000
0.034490000	0.079170000	0.095390000
0.173050000	0.043110000	0.095730000
0.268880000	0.094670000	0.012910000
0.402250000	0.272770000	0.011810000
0.350540000	0.178850000	0.096370000
0.414520000	0.372000000	0.255720000
0.343010000	0.392740000	0.178220000
0.161790000	0.338500000	0.178850000
0.257520000	0.385510000	0.262160000
0.078570000	0.255970000	0.261960000
0.031860000	0.160530000	0.178650000
0.087040000	0.036340000	0.178900000
0.034290000	0.079010000	0.262160000
0.172840000	0.042950000	0.262410000
0.268110000	0.095570000	0.179270000
0.407580000	0.275320000	0.180120000
0.349830000	0.178790000	0.262550000
0.406630000	0.361200000	0.433460000
0.344570000	0.392940000	0.345070000
0.161860000	0.338070000	0.345160000
0.257400000	0.385370000	0.427960000
0.078600000	0.256030000	0.428630000
0.031690000	0.160450000	0.345420000
0.087050000	0.036360000	0.345680000

0.034420000	0.079130000	0.428940000
0.173100000	0.042990000	0.428980000
0.268460000	0.094860000	0.345660000
0.418220000	0.270450000	0.346330000
0.351940000	0.177060000	0.429160000
0.395810000	0.351170000	0.596800000
0.342430000	0.391790000	0.511650000
0.161820000	0.338590000	0.511570000
0.257210000	0.387430000	0.594670000
0.078850000	0.256310000	0.595290000
0.031880000	0.160620000	0.512160000
0.087590000	0.036860000	0.512390000
0.034770000	0.079400000	0.595620000
0.173560000	0.043300000	0.595670000
0.268800000	0.094030000	0.512120000
0.402950000	0.272700000	0.512070000
0.352150000	0.176240000	0.595450000
0.395420000	0.351560000	0.762220000
0.342290000	0.393420000	0.678520000
0.161610000	0.339410000	0.678310000
0.257120000	0.388820000	0.761630000
0.079020000	0.256510000	0.761950000
0.032190000	0.160870000	0.678800000
0.088090000	0.037310000	0.679000000
0.034960000	0.079560000	0.762180000
0.173890000	0.043550000	0.762380000
0.269370000	0.093240000	0.678920000
0.399990000	0.270990000	0.679240000
0.352780000	0.175370000	0.762490000
0.395580000	0.351780000	0.927550000

0.342240000	0.393930000	0.845000000
0.161510000	0.339690000	0.845200000
0.257050000	0.388610000	0.928600000
0.078980000	0.256470000	0.928630000
0.032320000	0.160950000	0.845380000
0.088100000	0.037320000	0.845540000
0.034810000	0.079440000	0.928730000
0.173660000	0.043470000	0.929100000
0.269440000	0.093320000	0.846030000
0.400120000	0.271210000	0.845370000
0.352470000	0.176270000	0.929520000
0.576480000	0.440870000	0.211140000
0.578200000	0.386510000	0.213910000
0.495950000	0.423600000	0.219320000
0.557360000	0.402730000	0.341340000
0.454110000	0.354100000	0.349390000
0.496260000	0.324010000	0.204040000
0.616100000	0.476000000	0.194990000
0.618610000	0.392670000	0.198990000

(13)　　*HNNH$_2$ adsorption on Mn$_4$/BNNT (6, 6) ($G = -171669.8609$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B	N	Mn	H
71	74	4	3

Direct

0.402250000	0.327450000	0.011790000
0.364380000	0.382120000	0.095320000
0.287700000	0.392510000	0.012790000

0.105760000	0.286420000	0.013100000
0.194530000	0.357940000	0.096460000
0.045180000	0.193500000	0.096480000
0.030480000	0.105630000	0.013240000
0.142460000	0.038010000	0.013520000
0.066380000	0.048300000	0.096720000
0.235760000	0.074950000	0.097310000
0.324420000	0.147970000	0.014530000
0.387880000	0.241240000	0.097720000
0.417520000	0.338650000	0.178330000
0.369000000	0.387090000	0.262150000
0.287980000	0.391050000	0.179500000
0.105700000	0.286070000	0.179800000
0.194890000	0.357070000	0.263080000
0.044880000	0.193300000	0.263140000
0.030210000	0.105410000	0.179950000
0.142050000	0.037670000	0.180360000
0.066200000	0.048150000	0.263550000
0.235670000	0.074910000	0.264020000
0.322990000	0.149260000	0.181170000
0.392420000	0.240320000	0.266550000
0.366960000	0.382180000	0.429900000
0.288650000	0.390090000	0.346130000
0.105590000	0.285890000	0.346310000
0.194810000	0.356990000	0.429260000
0.044860000	0.193360000	0.429830000
0.030130000	0.105380000	0.346700000
0.142130000	0.037700000	0.347120000
0.066490000	0.048440000	0.430310000
0.236100000	0.074340000	0.430290000

0.324490000	0.147950000	0.347290000
0.393950000	0.239110000	0.429920000
0.405070000	0.327990000	0.513320000
0.363230000	0.380570000	0.596340000
0.287820000	0.390490000	0.512480000
0.105660000	0.286150000	0.512870000
0.194570000	0.358080000	0.595880000
0.045130000	0.193600000	0.596510000
0.030340000	0.105590000	0.513410000
0.142650000	0.038140000	0.513720000
0.066970000	0.048880000	0.596930000
0.236550000	0.074000000	0.596920000
0.325150000	0.146730000	0.513280000
0.387560000	0.238850000	0.596240000
0.400450000	0.325150000	0.680330000
0.363250000	0.381830000	0.762680000
0.287780000	0.392610000	0.679180000
0.105760000	0.286510000	0.679570000
0.194420000	0.358900000	0.762700000
0.045380000	0.193770000	0.763170000
0.030610000	0.105800000	0.680030000
0.143070000	0.038490000	0.680330000
0.067150000	0.049030000	0.763460000
0.236810000	0.073860000	0.763760000
0.325770000	0.145900000	0.680150000
0.387010000	0.238130000	0.763550000
0.400600000	0.325760000	0.845910000
0.363300000	0.382080000	0.928900000
0.287790000	0.393390000	0.845960000
0.105810000	0.286620000	0.846340000

0.194400000	0.358840000	0.929620000
0.045400000	0.193710000	0.929820000
0.030660000	0.105820000	0.846620000
0.143030000	0.038460000	0.846890000
0.066850000	0.048750000	0.930000000
0.236480000	0.074310000	0.930640000
0.325700000	0.146040000	0.847480000
0.387390000	0.239150000	0.930460000
0.399330000	0.354170000	0.093850000
0.342650000	0.392900000	0.012450000
0.162170000	0.339640000	0.013070000
0.257700000	0.387110000	0.096440000
0.079200000	0.256790000	0.096370000
0.032250000	0.161350000	0.013110000
0.087050000	0.036920000	0.013380000
0.034290000	0.079590000	0.096580000
0.172460000	0.042970000	0.097030000
0.268290000	0.094470000	0.014290000
0.402370000	0.272510000	0.013320000
0.349880000	0.178600000	0.097830000
0.415290000	0.372510000	0.256860000
0.343660000	0.392960000	0.179150000
0.162390000	0.338890000	0.179820000
0.258090000	0.385660000	0.263100000
0.078930000	0.256570000	0.263000000
0.031950000	0.161110000	0.179770000
0.086590000	0.036500000	0.180160000
0.034110000	0.079470000	0.263360000
0.172300000	0.042840000	0.263720000
0.267540000	0.095220000	0.180620000

0.406960000	0.274940000	0.181850000
0.349480000	0.178290000	0.263940000
0.405800000	0.359200000	0.433840000
0.344820000	0.392510000	0.346030000
0.162400000	0.338460000	0.346140000
0.257870000	0.385300000	0.428950000
0.078910000	0.256620000	0.429680000
0.031750000	0.161040000	0.346530000
0.086680000	0.036610000	0.346950000
0.034240000	0.079600000	0.430130000
0.172650000	0.043020000	0.430290000
0.268010000	0.094370000	0.346970000
0.418790000	0.269560000	0.347760000
0.352040000	0.176120000	0.430460000
0.395980000	0.350280000	0.597550000
0.342550000	0.390890000	0.512520000
0.162320000	0.338950000	0.512590000
0.257720000	0.387270000	0.595640000
0.079140000	0.256890000	0.596370000
0.031910000	0.161210000	0.513280000
0.087260000	0.037170000	0.513640000
0.034570000	0.079860000	0.596790000
0.173140000	0.043370000	0.596980000
0.268410000	0.093590000	0.513470000
0.403400000	0.271740000	0.513380000
0.352160000	0.175410000	0.596860000
0.395820000	0.351070000	0.763130000
0.342630000	0.392790000	0.679340000
0.162160000	0.339720000	0.679350000
0.257710000	0.388690000	0.762560000

0.079350000	0.257070000	0.763040000
0.032210000	0.161440000	0.679930000
0.087720000	0.037580000	0.680230000
0.034730000	0.079980000	0.763360000
0.173410000	0.043580000	0.763690000
0.268930000	0.092910000	0.680330000
0.400210000	0.270290000	0.680520000
0.352590000	0.174800000	0.763960000
0.396160000	0.351650000	0.928560000
0.342790000	0.393690000	0.845850000
0.162120000	0.339990000	0.846210000
0.257690000	0.388620000	0.929520000
0.079360000	0.257020000	0.929700000
0.032370000	0.161500000	0.846510000
0.087660000	0.037500000	0.846770000
0.034590000	0.079850000	0.929910000
0.173100000	0.043410000	0.930400000
0.268920000	0.093100000	0.847440000
0.400390000	0.270770000	0.846730000
0.352070000	0.175940000	0.931020000
0.579780000	0.438110000	0.209840000
0.578330000	0.391640000	0.151760000
0.497510000	0.421770000	0.222240000
0.560470000	0.399740000	0.342700000
0.454270000	0.353500000	0.349070000
0.496870000	0.324120000	0.199420000
0.615700000	0.477350000	0.193050000
0.615000000	0.388430000	0.162470000
0.577260000	0.401170000	0.084490000

(14) *HN adsorption on Mn$_4$/BNNT (6, 6) ($G = -170149.2617$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B	N	Mn	H
71	73	4	1

Direct

0.401800000	0.327770000	0.012020000
0.363580000	0.382340000	0.095460000
0.287180000	0.392980000	0.012970000
0.105420000	0.286640000	0.013410000
0.194070000	0.358350000	0.096740000
0.045090000	0.193640000	0.096840000
0.030690000	0.105890000	0.013660000
0.143160000	0.038860000	0.014090000
0.066860000	0.048810000	0.097190000
0.236510000	0.076220000	0.097950000
0.325180000	0.149010000	0.015150000
0.389000000	0.242310000	0.098210000
0.418220000	0.340390000	0.178120000
0.369160000	0.388230000	0.262000000
0.287580000	0.391620000	0.179720000
0.105370000	0.286250000	0.180140000
0.194500000	0.357370000	0.263390000
0.044750000	0.193400000	0.263510000
0.030390000	0.105640000	0.180370000
0.142750000	0.038600000	0.180890000
0.066690000	0.048670000	0.264040000
0.236400000	0.076170000	0.264540000
0.323840000	0.150630000	0.181830000

0.394400000	0.241500000	0.267250000
0.366700000	0.382530000	0.429930000
0.288360000	0.390390000	0.346310000
0.105260000	0.286020000	0.346630000
0.194470000	0.357110000	0.429530000
0.044710000	0.193450000	0.430210000
0.030310000	0.105610000	0.347140000
0.142840000	0.038570000	0.347630000
0.067050000	0.048990000	0.430810000
0.236850000	0.075160000	0.430790000
0.325320000	0.148970000	0.347820000
0.394290000	0.239470000	0.431090000
0.404840000	0.328220000	0.513920000
0.363010000	0.380930000	0.596610000
0.287510000	0.390640000	0.512670000
0.105340000	0.286260000	0.513180000
0.194230000	0.358230000	0.596110000
0.044990000	0.193700000	0.596890000
0.030560000	0.105830000	0.513850000
0.143380000	0.038870000	0.514230000
0.067570000	0.049430000	0.597420000
0.237220000	0.074490000	0.597540000
0.325820000	0.147130000	0.514040000
0.387740000	0.239320000	0.597100000
0.400390000	0.325680000	0.680790000
0.362940000	0.382190000	0.762970000
0.287450000	0.392860000	0.679390000
0.105430000	0.286660000	0.679860000
0.194030000	0.359170000	0.762920000
0.045270000	0.193900000	0.763540000

0.030870000	0.106060000	0.680470000
0.143750000	0.039150000	0.680880000
0.067740000	0.049580000	0.763940000
0.237480000	0.074450000	0.764430000
0.326400000	0.146400000	0.680880000
0.387360000	0.238800000	0.764160000
0.400490000	0.326290000	0.846290000
0.362690000	0.382280000	0.929140000
0.287360000	0.393760000	0.846160000
0.105460000	0.286820000	0.846630000
0.193940000	0.359230000	0.929840000
0.045310000	0.193870000	0.930190000
0.030920000	0.106100000	0.847040000
0.143710000	0.039180000	0.847470000
0.067390000	0.049270000	0.930480000
0.237190000	0.075190000	0.931320000
0.326400000	0.146740000	0.848150000
0.388050000	0.239980000	0.930880000
0.398030000	0.353900000	0.094170000
0.341990000	0.393130000	0.012610000
0.161740000	0.340000000	0.013340000
0.257270000	0.387650000	0.096700000
0.078960000	0.256950000	0.096700000
0.032280000	0.161520000	0.013480000
0.087660000	0.037560000	0.013880000
0.034580000	0.079900000	0.097010000
0.173230000	0.044050000	0.097620000
0.269030000	0.095600000	0.014950000
0.403150000	0.273460000	0.013700000
0.350730000	0.179790000	0.098430000

0.416380000	0.374910000	0.256420000
0.343350000	0.393680000	0.179320000
0.162000000	0.339190000	0.180150000
0.257760000	0.386080000	0.263400000
0.078680000	0.256690000	0.263330000
0.031940000	0.161260000	0.180150000
0.087170000	0.037140000	0.180660000
0.034390000	0.079760000	0.263800000
0.173070000	0.043910000	0.264230000
0.268300000	0.096750000	0.181240000
0.409590000	0.276400000	0.182110000
0.350540000	0.179700000	0.264600000
0.405490000	0.359250000	0.433970000
0.344710000	0.392980000	0.346110000
0.162060000	0.338640000	0.346450000
0.257560000	0.385380000	0.429150000
0.078630000	0.256730000	0.430000000
0.031710000	0.161160000	0.346910000
0.087320000	0.037270000	0.347440000
0.034590000	0.079920000	0.430580000
0.173410000	0.043880000	0.430770000
0.268780000	0.095550000	0.347460000
0.419830000	0.270010000	0.349410000
0.352770000	0.176600000	0.431280000
0.395860000	0.350730000	0.597870000
0.342330000	0.391100000	0.512620000
0.162010000	0.339070000	0.512840000
0.257410000	0.387410000	0.595790000
0.078860000	0.257000000	0.596680000
0.031870000	0.161320000	0.513660000

0.087970000	0.037850000	0.514120000
0.034980000	0.080210000	0.597240000
0.173830000	0.044020000	0.597520000
0.269120000	0.094060000	0.514070000
0.403330000	0.272160000	0.514230000
0.352770000	0.175900000	0.597600000
0.395610000	0.351550000	0.763490000
0.342340000	0.393100000	0.679520000
0.161820000	0.339910000	0.679560000
0.257330000	0.388990000	0.762700000
0.079080000	0.257210000	0.763350000
0.032200000	0.161570000	0.680310000
0.088420000	0.038240000	0.680730000
0.035150000	0.080340000	0.763790000
0.174100000	0.044260000	0.764280000
0.269610000	0.093380000	0.680980000
0.400310000	0.270900000	0.681120000
0.353210000	0.175460000	0.764600000
0.395490000	0.351820000	0.928920000
0.342310000	0.393960000	0.846050000
0.161720000	0.340280000	0.846420000
0.257240000	0.389080000	0.929680000
0.079100000	0.257190000	0.930020000
0.032390000	0.161660000	0.846890000
0.088320000	0.038150000	0.847280000
0.034950000	0.080180000	0.930340000
0.173830000	0.044270000	0.931010000
0.269630000	0.093830000	0.848110000
0.400650000	0.271500000	0.847180000
0.352850000	0.176790000	0.931610000

0.564470000	0.409690000	0.202490000
0.499430000	0.423540000	0.221490000
0.558840000	0.392400000	0.333410000
0.453230000	0.353090000	0.349310000
0.499380000	0.330440000	0.184450000
0.602070000	0.432750000	0.165720000

(15)　　$^*H_2N$ adsorption on Mn_4/BNNT (6, 6) ($G = -170165.3597$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B	N	Mn	H
71	73	4	2

Direct

0.402880000	0.323230000	0.012420000
0.366930000	0.379760000	0.095640000
0.291850000	0.392370000	0.013060000
0.109560000	0.289450000	0.013630000
0.199100000	0.359510000	0.096910000
0.047350000	0.196930000	0.097090000
0.030910000	0.108470000	0.013940000
0.140340000	0.037920000	0.014490000
0.065220000	0.049790000	0.097540000
0.233460000	0.073320000	0.098430000
0.322910000	0.144490000	0.015660000
0.388230000	0.237190000	0.098980000
0.419630000	0.335640000	0.178750000
0.373370000	0.386110000	0.262100000
0.292350000	0.391040000	0.179900000
0.109490000	0.289040000	0.180330000

0.199480000	0.358510000	0.263520000
0.046990000	0.196710000	0.263750000
0.030610000	0.108240000	0.180660000
0.139960000	0.037710000	0.181300000
0.065080000	0.049700000	0.264390000
0.233400000	0.073290000	0.265000000
0.321760000	0.146170000	0.182440000
0.394790000	0.236240000	0.267950000
0.369390000	0.379160000	0.429940000
0.293060000	0.389820000	0.346350000
0.109340000	0.288830000	0.346800000
0.199390000	0.358290000	0.429630000
0.046960000	0.196790000	0.430440000
0.030570000	0.108250000	0.347430000
0.140100000	0.037730000	0.348030000
0.065480000	0.050060000	0.431150000
0.233870000	0.072310000	0.431170000
0.323480000	0.144240000	0.348190000
0.394500000	0.233670000	0.431220000
0.405290000	0.322530000	0.513800000
0.365930000	0.377610000	0.596590000
0.291950000	0.389890000	0.512800000
0.109390000	0.289130000	0.513360000
0.199100000	0.359500000	0.596260000
0.047260000	0.197050000	0.597130000
0.030860000	0.108490000	0.514140000
0.140650000	0.038030000	0.514590000
0.066000000	0.050480000	0.597740000
0.234180000	0.071620000	0.597940000
0.323900000	0.142260000	0.514440000

0.387560000	0.233840000	0.597460000
0.401640000	0.320890000	0.680850000
0.366170000	0.379210000	0.763000000
0.291970000	0.392060000	0.679480000
0.109480000	0.289530000	0.680070000
0.198960000	0.360430000	0.763070000
0.047550000	0.197220000	0.763790000
0.031150000	0.108710000	0.680750000
0.140980000	0.038240000	0.681240000
0.066130000	0.050560000	0.764260000
0.234370000	0.071570000	0.764840000
0.324320000	0.141600000	0.681360000
0.386920000	0.233530000	0.764580000
0.401930000	0.321820000	0.846480000
0.366090000	0.379620000	0.929240000
0.291990000	0.393050000	0.846240000
0.109560000	0.289660000	0.846840000
0.198930000	0.360460000	0.930000000
0.047590000	0.197160000	0.930440000
0.031170000	0.108690000	0.847320000
0.140890000	0.038220000	0.847840000
0.065740000	0.050230000	0.930810000
0.234070000	0.072290000	0.931750000
0.324150000	0.142100000	0.848630000
0.387470000	0.234830000	0.931350000
0.399660000	0.349580000	0.094580000
0.346020000	0.391250000	0.012650000
0.166700000	0.341790000	0.013520000
0.262230000	0.387610000	0.096860000
0.082560000	0.260160000	0.096900000

0.033850000	0.164730000	0.013730000
0.085450000	0.037870000	0.014240000
0.034140000	0.082090000	0.097310000
0.170200000	0.042520000	0.098020000
0.266010000	0.092030000	0.015390000
0.403090000	0.268340000	0.014230000
0.348960000	0.174920000	0.098950000
0.419950000	0.371740000	0.256390000
0.347620000	0.392020000	0.179540000
0.166950000	0.340900000	0.180300000
0.262660000	0.386080000	0.263490000
0.082220000	0.259920000	0.263520000
0.033480000	0.164480000	0.180400000
0.084990000	0.037500000	0.181020000
0.033980000	0.082000000	0.264110000
0.170070000	0.042430000	0.264640000
0.265380000	0.093190000	0.181700000
0.409920000	0.271290000	0.182760000
0.349230000	0.174790000	0.265030000
0.405720000	0.353220000	0.433640000
0.348840000	0.391210000	0.346080000
0.166960000	0.340340000	0.346560000
0.262380000	0.385330000	0.429200000
0.082160000	0.259990000	0.430190000
0.033260000	0.164410000	0.347160000
0.085180000	0.037680000	0.347800000
0.034210000	0.082190000	0.430880000
0.170460000	0.042450000	0.431150000
0.265900000	0.092000000	0.347850000
0.421220000	0.263990000	0.349990000

0.351530000	0.171140000	0.431690000
0.397360000	0.345950000	0.597750000
0.345920000	0.388720000	0.512770000
0.166860000	0.340890000	0.512970000
0.262200000	0.387410000	0.595940000
0.082390000	0.260280000	0.596880000
0.033460000	0.164600000	0.513920000
0.085860000	0.038270000	0.514450000
0.034610000	0.082470000	0.597530000
0.170850000	0.042540000	0.597900000
0.266170000	0.090510000	0.514490000
0.403850000	0.266560000	0.514510000
0.351400000	0.170510000	0.598070000
0.397700000	0.347370000	0.763540000
0.346060000	0.390690000	0.679570000
0.166660000	0.341800000	0.679730000
0.262190000	0.388930000	0.762830000
0.082640000	0.260460000	0.763570000
0.033810000	0.164830000	0.680560000
0.086270000	0.038600000	0.681050000
0.034740000	0.082560000	0.764070000
0.171060000	0.042700000	0.764660000
0.266590000	0.089820000	0.681430000
0.400500000	0.265590000	0.681440000
0.351610000	0.170280000	0.765120000
0.397740000	0.347930000	0.929130000
0.346250000	0.391830000	0.846080000
0.166620000	0.342150000	0.846610000
0.262170000	0.389090000	0.929780000
0.082700000	0.260410000	0.930240000

0.033990000	0.164890000	0.847140000
0.086130000	0.038450000	0.847610000
0.034510000	0.082370000	0.930630000
0.170760000	0.042670000	0.931400000
0.266550000	0.090310000	0.848550000
0.400830000	0.266410000	0.847590000
0.351050000	0.171800000	0.932120000
0.553040000	0.406970000	0.122450000
0.503130000	0.417880000	0.217060000
0.560120000	0.380710000	0.335920000
0.454580000	0.348080000	0.350000000
0.499830000	0.325330000	0.168250000
0.597000000	0.425480000	0.132370000
0.546560000	0.414470000	0.056250000

(16) $^*H_3N$ adsorption on Mn_4/BNNT (6, 6) ($G = -170181.0171$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B	N	Mn	H
71	73	4	3

Direct

0.405440000	0.329540000	0.013830000
0.367600000	0.384080000	0.097210000
0.290820000	0.394420000	0.014650000
0.108520000	0.289780000	0.015040000
0.197730000	0.360500000	0.098340000
0.047100000	0.197090000	0.098460000
0.031580000	0.108950000	0.015260000
0.142730000	0.040440000	0.015570000

0.066920000	0.051130000	0.098770000
0.235910000	0.076980000	0.099470000
0.324770000	0.149730000	0.016850000
0.388530000	0.242900000	0.100790000
0.420670000	0.340440000	0.180960000
0.372330000	0.389190000	0.264040000
0.291080000	0.392890000	0.181330000
0.108510000	0.289420000	0.181740000
0.198160000	0.359670000	0.264980000
0.046820000	0.196900000	0.265110000
0.031350000	0.108740000	0.181970000
0.142280000	0.040020000	0.182480000
0.066770000	0.051010000	0.265630000
0.235870000	0.076830000	0.266190000
0.323180000	0.151010000	0.183480000
0.394250000	0.241600000	0.268710000
0.369940000	0.383890000	0.431730000
0.291960000	0.392350000	0.348010000
0.108410000	0.289270000	0.348230000
0.198040000	0.359650000	0.431130000
0.046790000	0.196990000	0.431790000
0.031270000	0.108740000	0.348710000
0.142450000	0.040160000	0.349260000
0.067120000	0.051390000	0.432380000
0.236460000	0.076370000	0.432400000
0.325220000	0.149310000	0.349340000
0.396630000	0.239800000	0.431510000
0.406970000	0.328610000	0.514830000
0.365710000	0.381710000	0.598110000
0.290890000	0.392530000	0.514330000

0.108450000	0.289550000	0.514780000
0.197730000	0.360760000	0.597770000
0.047040000	0.197230000	0.598470000
0.031470000	0.108960000	0.515410000
0.143110000	0.040800000	0.515820000
0.067630000	0.051880000	0.598970000
0.236980000	0.076180000	0.599010000
0.326120000	0.147970000	0.515270000
0.389650000	0.239750000	0.598050000
0.402700000	0.326090000	0.682090000
0.365960000	0.383220000	0.764450000
0.290790000	0.394540000	0.681040000
0.108510000	0.289910000	0.681500000
0.197570000	0.361560000	0.764610000
0.047270000	0.197380000	0.765140000
0.031710000	0.109170000	0.682030000
0.143540000	0.041200000	0.682390000
0.067790000	0.052010000	0.765480000
0.237200000	0.076080000	0.765860000
0.326750000	0.147210000	0.682250000
0.389000000	0.239190000	0.765570000
0.403240000	0.327140000	0.847730000
0.366240000	0.383790000	0.930700000
0.290840000	0.395330000	0.847810000
0.108550000	0.290000000	0.848280000
0.197580000	0.361450000	0.931530000
0.047290000	0.197310000	0.931800000
0.031760000	0.109170000	0.848620000
0.143420000	0.041080000	0.848930000
0.067420000	0.051640000	0.932020000

0.236740000	0.076470000	0.932760000
0.326420000	0.147570000	0.849680000
0.389160000	0.240480000	0.932690000
0.403170000	0.356670000	0.095650000
0.345730000	0.394690000	0.014260000
0.165330000	0.342500000	0.014970000
0.260850000	0.389130000	0.098260000
0.081730000	0.260340000	0.098320000
0.033850000	0.164900000	0.015090000
0.087460000	0.039610000	0.015400000
0.035180000	0.082770000	0.098600000
0.172630000	0.045200000	0.099100000
0.268520000	0.096460000	0.016450000
0.405490000	0.274220000	0.015640000
0.350120000	0.180350000	0.100090000
0.418600000	0.375110000	0.258500000
0.346570000	0.394560000	0.180900000
0.165610000	0.341700000	0.181730000
0.261320000	0.387840000	0.264970000
0.081470000	0.260130000	0.264940000
0.033570000	0.164670000	0.181760000
0.086980000	0.039160000	0.182230000
0.035020000	0.082670000	0.265390000
0.172500000	0.045050000	0.265840000
0.267670000	0.097080000	0.182750000
0.407390000	0.276220000	0.184440000
0.350070000	0.179750000	0.266090000
0.408010000	0.359990000	0.435520000
0.348160000	0.394870000	0.347970000
0.165610000	0.341310000	0.348030000

0.261070000	0.387590000	0.430790000
0.081440000	0.260210000	0.431610000
0.033380000	0.164620000	0.348510000
0.087150000	0.039350000	0.349050000
0.035160000	0.082830000	0.432160000
0.173010000	0.045460000	0.432410000
0.268340000	0.096100000	0.349060000
0.422710000	0.269900000	0.349610000
0.353310000	0.177050000	0.432450000
0.397930000	0.350890000	0.599250000
0.345390000	0.392470000	0.514370000
0.165490000	0.341850000	0.514460000
0.260840000	0.389460000	0.597510000
0.081650000	0.260480000	0.598290000
0.033510000	0.164800000	0.515250000
0.087830000	0.040040000	0.515710000
0.035470000	0.083100000	0.598810000
0.173590000	0.045990000	0.599080000
0.268860000	0.095470000	0.515570000
0.406050000	0.272620000	0.515120000
0.353530000	0.176360000	0.598920000
0.398340000	0.352230000	0.764880000
0.345390000	0.394230000	0.681170000
0.165290000	0.342660000	0.681250000
0.260840000	0.390850000	0.764440000
0.081860000	0.260640000	0.764980000
0.033800000	0.165020000	0.681900000
0.088300000	0.040480000	0.682280000
0.035620000	0.083200000	0.765360000
0.173840000	0.046170000	0.765760000

0.269400000	0.094880000	0.682470000
0.402520000	0.271240000	0.682460000
0.353840000	0.175910000	0.766190000
0.399030000	0.353220000	0.930340000
0.345700000	0.395300000	0.847630000
0.165270000	0.342900000	0.848130000
0.260850000	0.390680000	0.931390000
0.081860000	0.260570000	0.931650000
0.033950000	0.165070000	0.848490000
0.088170000	0.040320000	0.848790000
0.035460000	0.083040000	0.931920000
0.173410000	0.045840000	0.932460000
0.269300000	0.095160000	0.849620000
0.402930000	0.272030000	0.848810000
0.352880000	0.177450000	0.933360000
0.534470000	0.315860000	0.076900000
0.501260000	0.424630000	0.218400000
0.568630000	0.408090000	0.319790000
0.458110000	0.355360000	0.350840000
0.501950000	0.328750000	0.203420000
0.545670000	0.284030000	0.074930000
0.501070000	0.304660000	0.031090000
0.569800000	0.353840000	0.055400000

(17)   the second $^*H_3N$ desorption on Mn$_4$/BNNT (6, 6) ($G = -170179.4254$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B   N   Mn   H

71   73   4   3

Direct

0.405950000	0.327830000	0.013470000
0.369030000	0.383190000	0.097470000
0.293180000	0.395110000	0.014970000
0.110630000	0.292390000	0.015050000
0.200200000	0.362220000	0.098510000
0.048290000	0.200040000	0.098450000
0.031420000	0.111410000	0.014990000
0.141160000	0.041090000	0.015120000
0.066090000	0.053000000	0.098430000
0.234250000	0.076180000	0.098800000
0.323670000	0.147660000	0.015800000
0.388710000	0.240270000	0.098830000
0.419960000	0.337290000	0.180410000
0.373050000	0.387370000	0.264510000
0.293230000	0.393320000	0.181600000
0.110510000	0.292050000	0.181820000
0.200540000	0.361370000	0.265130000
0.047750000	0.199780000	0.265050000
0.031180000	0.111230000	0.181850000
0.140750000	0.040810000	0.181960000
0.065750000	0.052770000	0.265230000
0.234120000	0.076330000	0.265560000
0.322390000	0.148990000	0.182540000
0.393090000	0.239500000	0.267680000
0.372010000	0.384720000	0.432260000
0.294120000	0.393120000	0.348250000
0.110410000	0.291890000	0.348280000
0.200520000	0.361520000	0.431290000
0.047850000	0.199860000	0.431700000

0.031050000	0.111190000	0.348470000
0.140710000	0.040810000	0.348710000
0.065880000	0.052920000	0.431970000
0.234400000	0.076050000	0.431860000
0.323570000	0.148170000	0.348830000
0.394370000	0.239020000	0.431240000
0.408040000	0.328730000	0.515460000
0.367990000	0.382790000	0.598580000
0.293380000	0.393970000	0.514610000
0.110580000	0.292180000	0.514830000
0.200320000	0.362680000	0.597940000
0.048200000	0.200110000	0.598360000
0.031340000	0.111400000	0.515170000
0.141140000	0.041190000	0.515320000
0.066330000	0.053300000	0.598620000
0.234830000	0.075760000	0.598440000
0.324080000	0.147290000	0.514770000
0.388420000	0.238750000	0.597740000
0.403410000	0.325610000	0.682310000
0.368020000	0.383700000	0.764840000
0.293360000	0.395960000	0.681370000
0.110710000	0.292520000	0.681530000
0.200200000	0.363440000	0.764800000
0.048380000	0.200240000	0.765020000
0.031620000	0.111620000	0.681800000
0.141570000	0.041500000	0.681930000
0.066590000	0.053510000	0.765170000
0.235120000	0.075430000	0.765210000
0.324830000	0.146190000	0.681560000
0.387950000	0.237760000	0.765050000

0.403800000	0.326120000	0.847750000
0.368130000	0.383670000	0.931010000
0.293370000	0.396430000	0.848160000
0.110730000	0.292600000	0.848290000
0.200170000	0.363240000	0.931700000
0.048350000	0.200200000	0.931650000
0.031640000	0.111630000	0.848390000
0.141620000	0.041480000	0.848490000
0.066450000	0.053350000	0.931710000
0.234860000	0.075630000	0.932070000
0.324840000	0.146020000	0.848810000
0.388270000	0.238560000	0.931860000
0.404020000	0.355090000	0.095830000
0.347710000	0.394570000	0.014710000
0.167850000	0.344560000	0.015090000
0.263290000	0.390090000	0.098540000
0.083560000	0.263200000	0.098310000
0.034390000	0.167740000	0.015010000
0.086280000	0.041100000	0.015070000
0.034740000	0.085070000	0.098370000
0.170970000	0.045560000	0.098620000
0.266800000	0.095070000	0.015700000
0.403890000	0.271850000	0.014780000
0.349730000	0.177830000	0.099150000
0.417710000	0.370760000	0.259170000
0.348170000	0.393720000	0.181310000
0.168030000	0.343760000	0.181860000
0.263650000	0.388740000	0.265180000
0.083200000	0.262990000	0.264970000
0.034270000	0.167550000	0.181600000

0.085830000	0.040710000	0.181830000
0.034610000	0.085010000	0.265110000
0.170790000	0.045500000	0.265340000
0.266140000	0.095870000	0.182150000
0.408460000	0.273690000	0.182820000
0.349310000	0.177820000	0.265360000
0.410450000	0.361140000	0.436420000
0.349930000	0.394720000	0.348230000
0.168050000	0.343370000	0.348190000
0.263560000	0.388980000	0.431030000
0.083270000	0.263060000	0.431660000
0.034050000	0.167480000	0.348390000
0.085750000	0.040670000	0.348600000
0.034640000	0.085070000	0.431870000
0.171020000	0.045670000	0.431910000
0.266470000	0.095460000	0.348580000
0.419720000	0.269230000	0.348790000
0.351360000	0.176420000	0.431890000
0.399540000	0.351260000	0.599680000
0.347880000	0.393800000	0.514740000
0.168040000	0.343980000	0.514630000
0.263450000	0.391020000	0.597780000
0.083590000	0.263310000	0.598320000
0.034270000	0.167650000	0.515140000
0.086200000	0.041090000	0.515300000
0.034960000	0.085310000	0.598560000
0.171480000	0.046000000	0.598560000
0.266760000	0.095000000	0.514990000
0.405040000	0.271840000	0.514820000
0.351630000	0.175500000	0.598250000

0.399530000	0.351880000	0.765100000
0.347830000	0.395360000	0.681590000
0.167910000	0.344770000	0.681410000
0.263460000	0.392300000	0.764770000
0.083790000	0.263450000	0.764980000
0.034550000	0.167860000	0.681780000
0.086690000	0.041520000	0.681930000
0.035130000	0.085440000	0.765150000
0.171780000	0.046150000	0.765240000
0.267290000	0.094170000	0.681760000
0.401860000	0.270120000	0.682080000
0.352210000	0.174520000	0.765350000
0.400220000	0.352430000	0.930470000
0.347960000	0.395870000	0.848100000
0.167860000	0.344960000	0.848270000
0.263420000	0.391880000	0.931720000
0.083730000	0.263380000	0.931630000
0.034520000	0.167870000	0.848390000
0.086760000	0.041560000	0.848470000
0.035040000	0.085330000	0.931700000
0.171540000	0.045930000	0.931940000
0.267330000	0.094050000	0.848820000
0.401970000	0.270350000	0.848260000
0.351650000	0.175470000	0.932390000
0.898350000	0.055450000	0.083290000
0.501060000	0.419740000	0.218170000
0.565860000	0.401710000	0.325240000
0.457840000	0.353910000	0.351590000
0.499430000	0.323150000	0.208620000
0.921510000	0.034040000	0.082760000

0.870350000	0.039850000	0.029450000
0.927680000	0.098100000	0.069060000

(18)   the NH$_4^+$ formation on Mn$_4$/BNNT (6, 6) ($G = -174352.1471$ eV)

1.0

26.4829998016	0.0000000000	0.0000000000
-13.2414999008	22.9349505966	0.0000000000
0.0000000000	0.0000000000	14.7571001053

B	N	Mn	H	O
71	73	4	8	2

Direct

0.404990000	0.327360000	0.014520000
0.368590000	0.382930000	0.097990000
0.292370000	0.394440000	0.015590000
0.110040000	0.290750000	0.015880000
0.199530000	0.360890000	0.099290000
0.048140000	0.198230000	0.099220000
0.031990000	0.110000000	0.015960000
0.141380000	0.039390000	0.016040000
0.066340000	0.051250000	0.099300000
0.234400000	0.074840000	0.099820000
0.323610000	0.147240000	0.017170000
0.387320000	0.240340000	0.100970000
0.421110000	0.338500000	0.181070000
0.374660000	0.388610000	0.264550000
0.292940000	0.392650000	0.182210000
0.110120000	0.290240000	0.182620000
0.200180000	0.359820000	0.265870000
0.047810000	0.197920000	0.265870000
0.031660000	0.109640000	0.182590000
0.140820000	0.038860000	0.182900000

0.065920000	0.050960000	0.266090000
0.234180000	0.074920000	0.266610000
0.321880000	0.148510000	0.183740000
0.392180000	0.239570000	0.268910000
0.372340000	0.384690000	0.432910000
0.294310000	0.392620000	0.348790000
0.110190000	0.289970000	0.349060000
0.200150000	0.360020000	0.431880000
0.047910000	0.197940000	0.432570000
0.031320000	0.109440000	0.349360000
0.140820000	0.039060000	0.349730000
0.066040000	0.051210000	0.432910000
0.234590000	0.075040000	0.432920000
0.323170000	0.147810000	0.349810000
0.395010000	0.239190000	0.431170000
0.408010000	0.328770000	0.515840000
0.366920000	0.381770000	0.599360000
0.292820000	0.393170000	0.515300000
0.110380000	0.290290000	0.515540000
0.199610000	0.361470000	0.598590000
0.048310000	0.198240000	0.599260000
0.031760000	0.109790000	0.516130000
0.141420000	0.039840000	0.516380000
0.066490000	0.051610000	0.599610000
0.235230000	0.075170000	0.599470000
0.324070000	0.147200000	0.515560000
0.388500000	0.238660000	0.598290000
0.402450000	0.324840000	0.683250000
0.366790000	0.382700000	0.765620000
0.292420000	0.395200000	0.682090000

0.110320000	0.290790000	0.682270000
0.199270000	0.362380000	0.765520000
0.048470000	0.198440000	0.765790000
0.031380000	0.109530000	0.682660000
0.141980000	0.040350000	0.682960000
0.066820000	0.051940000	0.766190000
0.235600000	0.074860000	0.766240000
0.325120000	0.146010000	0.682520000
0.387870000	0.237460000	0.766190000
0.402820000	0.325390000	0.848730000
0.367040000	0.382890000	0.931670000
0.292350000	0.395700000	0.848850000
0.110140000	0.290980000	0.849060000
0.199240000	0.362140000	0.932470000
0.048390000	0.198490000	0.932500000
0.032010000	0.109980000	0.849270000
0.142020000	0.040180000	0.849450000
0.066800000	0.051750000	0.932630000
0.235240000	0.074720000	0.933120000
0.325070000	0.145740000	0.850050000
0.388110000	0.238330000	0.933480000
0.403180000	0.354880000	0.096000000
0.347010000	0.394410000	0.015110000
0.166950000	0.343340000	0.015930000
0.262580000	0.389450000	0.099280000
0.082950000	0.261480000	0.099150000
0.034580000	0.166050000	0.015780000
0.086310000	0.039070000	0.015970000
0.035110000	0.083440000	0.099190000
0.171010000	0.043480000	0.099580000

0.267050000	0.093960000	0.016780000
0.403510000	0.271600000	0.016140000
0.349110000	0.177400000	0.100440000
0.419670000	0.373300000	0.258630000
0.348200000	0.394190000	0.181790000
0.167400000	0.342240000	0.182710000
0.263270000	0.387900000	0.265930000
0.082780000	0.261130000	0.265800000
0.034090000	0.165680000	0.182450000
0.085730000	0.038540000	0.182770000
0.034610000	0.083090000	0.265940000
0.170740000	0.043370000	0.266380000
0.266140000	0.094460000	0.183230000
0.405300000	0.273300000	0.184510000
0.348380000	0.177390000	0.266530000
0.410790000	0.361540000	0.437670000
0.350770000	0.395730000	0.348770000
0.167570000	0.341730000	0.348890000
0.263180000	0.388170000	0.431530000
0.082980000	0.261140000	0.432420000
0.033860000	0.165510000	0.349200000
0.085680000	0.038650000	0.349600000
0.034550000	0.083130000	0.432760000
0.171140000	0.043990000	0.432980000
0.266520000	0.094230000	0.349650000
0.420990000	0.268810000	0.349190000
0.350970000	0.176310000	0.432770000
0.398570000	0.350410000	0.600730000
0.347360000	0.393360000	0.515560000
0.167460000	0.342540000	0.515200000

0.262730000	0.390520000	0.598390000
0.083300000	0.261460000	0.599050000
0.034100000	0.165720000	0.515980000
0.086220000	0.039270000	0.516300000
0.034650000	0.083260000	0.599510000
0.171820000	0.044750000	0.599580000
0.267040000	0.094310000	0.516000000
0.405510000	0.271800000	0.515590000
0.351850000	0.175240000	0.599140000
0.398540000	0.351130000	0.765980000
0.346900000	0.394690000	0.682370000
0.167030000	0.343640000	0.682030000
0.262530000	0.391850000	0.765430000
0.083340000	0.261720000	0.765720000
0.034470000	0.165920000	0.682680000
0.086780000	0.039760000	0.682860000
0.035060000	0.083500000	0.766130000
0.172200000	0.044900000	0.766180000
0.267740000	0.093620000	0.682760000
0.401880000	0.269790000	0.683090000
0.352530000	0.174140000	0.766440000
0.399210000	0.351820000	0.931060000
0.346980000	0.395320000	0.848680000
0.166860000	0.343900000	0.849000000
0.262480000	0.391420000	0.932390000
0.083130000	0.261740000	0.932430000
0.034620000	0.166140000	0.849250000
0.086900000	0.039720000	0.849360000
0.035370000	0.083680000	0.932580000
0.171820000	0.044300000	0.932880000

0.267760000	0.093340000	0.849880000
0.401860000	0.270020000	0.849440000
0.351760000	0.175070000	0.933670000
0.576760000	0.340130000	0.026500000
0.503850000	0.418790000	0.211560000
0.570300000	0.404260000	0.322890000
0.461650000	0.356940000	0.352630000
0.498300000	0.320740000	0.213600000
0.577000000	0.344940000	0.957270000
0.555400000	0.296500000	0.041790000
0.555780000	0.359880000	0.057490000
0.620760000	0.361040000	0.052690000
0.709750000	0.420210000	0.049510000
0.755450000	0.337910000	0.138000000
0.698160000	0.374470000	0.125600000
0.744330000	0.357760000	0.229790000
0.683020000	0.399310000	0.099120000
0.723980000	0.334440000	0.176710000