

## Mechanisms of Ammonia and Hydrazine Synthesis on $\eta$ - $\text{Mn}_3\text{N}_2$ -(100) Surfaces

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Figure S1. Optimised structures of ligands and cluster-ligand models on  $\text{Mn}_3\text{N}$  using the B3LYP-D3/ECP-121G (Mn), aug-cc-pVTZ (N,H) method shown below

### A-cluster

0 1  
Mn -0.11483800 1.21994200 0.00000000  
Mn -0.11483800 -0.60974100 1.05701000  
Mn -0.11483800 -0.60974100 -1.05701000  
N 1.23040200 -0.00164300 0.00000000

### B-ligand

N 0.0000 0.0000 0.000000

### B-cluster-ligand

0 2  
Mn 1.19314500 0.90230800 0.00149500  
Mn 0.16212600 -1.35243000 0.00051700  
Mn -1.42699200 0.58837800 -0.00184000  
N 0.13428600 -0.24743000 -1.28509000  
N 0.12186000 -0.24634300 1.28447600

### C-ligand

0 1  
N 0.79906200 -1.61864500 0.00000000  
H 0.50112000 -2.59236600 0.00000000

### C-cluster-ligand

0 1  
Mn -1.25453000 0.63304300 0.00000000  
Mn 0.44331000 -0.21638900 1.07733000  
Mn 0.44331000 -0.21638900 -1.07733000  
N 0.44331000 1.27375100 0.00000000

N	0.79906200	-1.61864500	0.00000000
H	0.50112000	-2.59236600	0.00000000

**D-ligand**

1 1

N	-0.93259700	-1.88288500	0.00000000
H	-1.95053700	-1.88885400	0.00000000
H	-0.60814100	-2.85080200	0.00000000

**D-cluster-ligand**

1 1

Mn	0.02452500	1.82013300	0.00000000
Mn	0.02452500	-0.61055900	1.08736400
Mn	0.02452500	-0.61055900	-1.08736400
N	1.03535200	0.42064000	0.00000000
N	-0.93259700	-1.88288500	0.00000000
H	-1.95053700	-1.88885400	0.00000000
H	-0.60814100	-2.85080200	0.00000000

**E-ligand**

0 1

N	-1.72835900	-0.56788900	0.32205200
N	-2.43770800	0.35758600	0.41726100

**E-cluster-ligand**

0 1

Mn	-0.04501500	-1.16185400	-0.09791400
Mn	-0.54867200	0.92737200	-0.21341800
Mn	1.48617700	0.27322600	0.42764700
N	0.97860700	0.07193100	-1.15472200
N	-1.72835900	-0.56788900	0.32205200
N	-2.43770800	0.35758600	0.41726100

**F-ligand**

1 1

N	-2.91331500	0.52199700	-0.69145100
N	-2.06508900	-0.13618300	-0.17042000
H	-3.82443000	0.52697000	-0.20495900

**F-cluster-ligand**

1 1

Mn	0.43116300	1.19635300	0.18667500
Mn	-0.62817500	-0.87422100	0.30992700
Mn	1.50444200	-0.38722200	-0.56755100
N	0.85535600	-0.22863100	1.14453800
N	-2.91331500	0.52199700	-0.69145100
N	-2.06508900	-0.13618300	-0.17042000
H	-3.82443000	0.52697000	-0.20495900

**G-ligand**

0 1

N	1.69916400	-0.88767200	0.37473900
N	1.75959600	0.49326000	0.63680500
H	2.58473800	-1.36194000	0.53744800
H	2.38434700	0.72316900	1.40613000

**G-cluster-ligand**

0 1

Mn	0.40525800	1.20674400	-0.29841100
Mn	0.07118400	-1.20142600	-0.30987600

Mn	-1.41480900	0.07629100	0.56333000
N	-0.81732000	0.19420000	-1.12863700
N	1.69916400	-0.88767200	0.37473900
N	1.75959600	0.49326000	0.63680500
H	2.58473800	-1.36194000	0.53744800
H	2.38434700	0.72316900	1.40613000

**H-ligand**

l 1			
N	1.28760400	-1.29038200	0.64509900
N	1.74451900	-0.10669500	0.68134500
H	1.67398500	-1.95880900	1.31948700

**H-cluster-ligand**

l 1			
Mn	0.86693000	1.09434600	-0.13904500
Mn	-0.16662800	-1.05349500	-0.51071600
Mn	-1.47647300	0.26785000	0.51745800
N	-0.49922300	0.57440000	-1.04243000
N	1.28760400	-1.29038200	0.64509900
N	1.74451900	-0.10669500	0.68134500
H	1.67398500	-1.95880900	1.31948700

**I-ligand**

l 1			
N	1.56262100	-0.02728600	-0.28215400
N	2.45553400	0.18279900	0.90543800
H	3.07418300	-0.62193800	1.01634000
H	3.03310700	1.01358300	0.76712500
H	1.88877500	0.29616900	1.74989400

**I-cluster-ligand**

l 1			
Mn	0.07969600	1.01601100	-0.58489100
Mn	0.13873700	-1.16239100	-0.29991400
Mn	-1.31191200	0.13705400	0.82799400
N	-1.25516700	-0.22046500	-0.92515500
N	1.56262100	-0.02728600	-0.28215400
N	2.45553400	0.18279900	0.90543800
H	3.07418300	-0.62193800	1.01634000
H	3.03310700	1.01358300	0.76712500
H	1.88877500	0.29616900	1.74989400

Figure S2. Optimised structures of N<sub>2</sub>, HN=NH and N=NH on Mn<sub>3</sub>N<sub>2</sub>-(100) surface calculated with E<sub>cut</sub> = 600 eV, a 3x5x1 gamma-point MP grid and the revPBE functional

**N2 site 1**

```

1.0000000000000000
12.0322999999999993 0.0000000000000000 0.0000000000000000
-0.0000000007000000 8.0876000000000001 0.0000000000000000
-0.0000000022000000 -0.0000000022000000 26.0656999999999996
Mn N
48 34
Direct
0.5035115085559685 0.5044373258816357 0.5405051774589037

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0.1827743322602559 0.7544152949901730 0.6183069607762247  
0.8242308197462651 0.7544027733674938 0.6183449748083096  
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0.3322829553474431 0.7543289956843433 0.5401029578439526  
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0.5034873607202366 0.5043465483658436 0.3886214912060692  
0.0036384767581554 0.7542591485238147 0.3942079115281655  
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0.833998398762685 0.7542708410293314 0.4628907391348660  
0.1791066144434601 0.5043360230899046 0.3836651850402263  
0.8279506964156631 0.5041535959402031 0.3837759940992815  
0.6868404424837427 0.7543382785408917 0.3857443318760647  
0.3207444468642111 0.7543354327330993 0.3855645310147875  
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0.0035139256514831 0.5043686695964374 0.6117014460200606  
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0.1573642022262313 0.7543309649807803 0.3807532992469000  
0.1569613171035881 0.2542483485954867 0.3807783908310309  
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0.6113322812416763 0.2722323819008068 0.2743811337201514

**HN=NH site 1**

1.000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 2

**Direct**

0.5036304066460315 0.5042428525065421 0.5389960328967692  
0.0039343235785850 0.7527652522039094 0.5410435478859493  
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0.3263818322864896 0.5036864247474169 0.6179407561608211  
0.1839242384614958 0.7536122130857064 0.6168709817846357  
0.8241969814396956 0.7524271998321104 0.6171843053260820  
0.1731260654246833 0.5044367320115293 0.5399910709077403  
0.8344900986847208 0.5023771248852266 0.5393798692266665  
0.6756849251186722 0.7524473788131600 0.5393830259933917  
0.3324112474928544 0.7542092879040657 0.5391115949805799  
0.0043997230343865 0.5039989137864256 0.4599898940436085  
0.5036426032458677 0.7526005501255647 0.4618407482120603  
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0.3345446247441970 0.5045897062577309 0.4598937943025386

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0.1749151451447968 0.5061169078251336 0.3818882193077918  
0.8299727573173117 0.4992006303096497 0.3835259884206384  
0.6929905413067163 0.7530889649907332 0.3860491414636060  
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0.3411936631962441 0.5112967093700641 0.3798997670529512  
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0.8445794547058052 0.5027985549228705 0.4628883611618340  
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0.1562245719411875 0.7576924751614034 0.3792459573937407  
0.1574742634421422 0.2543936364350465 0.3797526633620334  
0.3439157326970047 0.0043385858675124 0.5378991009267313  
0.5183876135138478 0.3831324949837759 0.3126330896584787  
0.5985617741962941 0.2688118789731019 0.3135102242131875  
0.5955705164843771 0.1857381239702128 0.2837513938785878  
0.4668707359902178 0.3760371294201142 0.2812701031225939

**N2 site 2**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N

48 34

**Direct**

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0.0028631747720090 0.7500497148841521 0.5418993517407623  
0.6813776539845627 0.4999742461388552 0.6183152398469224  
0.3244914065827034 0.5000018134027293 0.6181267395284160  
0.1825492815510956 0.7499569118853565 0.6181521895402664  
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0.0029237885964701 0.5000616045806950 0.6119333841341928  
0.0029701132039259 -0.0000454237622866 0.6119133254018175  
0.6856648681510812 0.2495579124957838 0.3855253472643426  
0.3199440754854232 0.2500195654783641 0.3854799195948679  
0.5028997363784904 0.2499832454194248 0.6101490717876131

0.5029880263448206 -0.0000566553430714 0.5405607262081046  
0.0028525049132432 0.2500512727298788 0.5419043061509624  
0.6814550862305545 0.0000768745490884 0.6182983863837768  
0.3243818642500300 0.0000679482066460 0.6181330354578080  
0.1823715355161218 0.2500391313971596 0.6181769095536160  
0.8234456330708687 0.2500189405111992 0.6183717472947599  
0.1722581471408584 -0.0000173258075694 0.5407563286684504  
0.8335352572162228 0.0000729959555138 0.5409013711897293  
0.6740322961512383 0.2500003719903439 0.5401348685458898  
0.6741165999495330 0.5000377679001728 0.4620485317438934  
0.0029117657568446 0.0000229099263685 0.4615602707086052  
0.8272316536952644 0.0000759819039977 0.3837736400467814  
0.3317646754338836 0.2500083632002796 0.5399981502151556  
0.1786024271678546 0.0000400044011421 0.3836380099226391  
0.1725693220770957 0.2500299513256692 0.4628413617008222  
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0.0029133106810520 0.2501256210180154 0.3944187058880093  
0.5029732529062780 -0.0001475100753753 0.3883297797407502  
0.5030412725838781 0.2500015434835336 0.4618460779530085  
0.6742337732074070 0.0001078793215931 0.4621159230255776  
0.8439100739553612 0.7500339494954229 0.5398936549334538  
0.6584177671901790 0.7499999221630230 0.6216396181262615  
0.3472948700428503 0.7500400388341070 0.6215680014695825  
0.3433160135139247 0.5000403564133560 0.5389813956542961  
0.6625899927134744 0.4999847475325546 0.5390887320421586  
0.1618337234640267 0.7500202754908222 0.5397361091862239  
0.6623039584441710 0.7500939619519671 0.4627235930347007  
0.1621554403070414 0.5000364213795984 0.4638211743803356  
0.3436842810445610 0.7500107538024658 0.4625565143426270  
0.1591888387721461 0.5000491244980834 0.6226043409016216  
0.3446321574162883 0.5000423209578899 0.3802575039676346  
0.6612566431789889 0.5002440761022665 0.3807096806425335  
0.8493197907632231 0.7501813546298651 0.3810212101401297  
0.8436821685418645 0.4999328272153964 0.4639801379226848  
0.8466851710506886 0.5000373050326570 0.6226886772628262  
0.6623475236199821 0.2500882007046206 0.4627620019467714  
0.8493212879140248 0.2498924835001035 0.3812258001938296  
0.6612950637411474 0.9996747260815289 0.3804585554443692  
0.3447388263119402 -0.0000325104301904 0.3802556928747933  
0.3437095324004503 0.2500082242004578 0.4625941885066278  
0.1621201222934824 0.0000231529085893 0.4638002954541313  
0.8437630015340400 -0.0000594287602831 0.4639437486814301  
0.1618231782548383 0.2499889624855780 0.5397277960488817  
0.8438803518738535 0.2500429277455254 0.5398635989079432  
0.6625931718375455 -0.0000253022776567 0.5391452431096118  
0.6585427274671075 0.2500066086263180 0.6216584955071802  
0.3472454724626748 0.2500037153816937 0.6215565736517094  
0.1591364065054258 -0.0000455042572798 0.6226031006597834  
0.8467463600525866 -0.0000678158033693 0.6226926967622135  
0.1566983743228422 0.7500013532050613 0.3808397457630711  
0.1567288105535936 0.2500332309087385 0.3807824063937681



0.3433378363752412 0.0000057635392418 0.5389821693940416  
0.7253537375706565 0.3180687519210449 0.2609958330564133  
0.7819371234563628 0.4274903941374086 0.2587129670957291

**N2 site 3**

1.0000000000000000  
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-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N

48 34

**Direct**

0.5023930970447591 0.5005201578300663 0.5411308426828620  
0.0024051397156079 0.7503744100910912 0.5424794414223214  
0.6811038838612529 0.5004644870261468 0.6187882237658722  
0.3238212609555809 0.5004872982259534 0.6188162049580259  
0.1819092357098232 0.7504331757814687 0.6188649993740055  
0.8231315986902451 0.7504743984908141 0.6189381501775605  
0.1718197003764392 0.5004101690124909 0.5413723773238929  
0.8329257840727975 0.5004415671825452 0.5414444049452758  
0.6736826206932512 0.7505543371244247 0.5407092440501068  
0.3311586896448385 0.7504656629096168 0.5406077959635402  
0.0025233921279650 0.5003776064654719 0.4621925745235382  
0.5024683604181495 0.7506469028370889 0.4624648024431058  
0.5026457921742231 0.5002376556618052 0.3889932379313339  
0.0023017938416795 0.7503374657892545 0.3951612100217821  
0.3313843783300963 0.5005541025399750 0.4625311372246408  
0.1719255625166370 0.7503788739809543 0.4634188536072923  
0.8328797749385093 0.7505138834338140 0.4634386673642926  
0.1780957995704837 0.5004776863466851 0.3841591196447194  
0.8273852744373070 0.5001790872970016 0.3845625999867116  
0.6847508377092604 0.7509007794303493 0.3861219811505349  
0.3191073003512331 0.7504647650582782 0.3860926765521505  
0.5024626411204121 0.7504796089831953 0.6108632773076659  
0.0024379397567568 0.5004039878763894 0.6124455626048625  
0.0024971168574371 0.0005050453802146 0.6122479426829477  
0.6866532143321794 0.2504878054114556 0.3862214418145274  
0.3195567772344716 0.2504126191629368 0.3860732165722909  
0.5023581145226197 0.2504094283440410 0.6105582853727229  
0.5024060273880596 0.0004185257407684 0.5409723723608542  
0.0024446780144716 0.2505223989249763 0.5423072352313845  
0.6811537773553987 0.0004186181604418 0.6187371914541929  
0.3239255993670068 0.0004521778266754 0.6187419702704534  
0.1819102145573881 0.2504930080174066 0.6187387744400075  
0.8228519663651885 0.2503796951883478 0.6188079257959115  
0.1716662853674474 0.0004942642034798 0.5412998872230821  
0.8330972045282348 0.0003871231112682 0.5413375742782951  
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0.6737074618345488 0.0005473959681322 0.4625438361121170  
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0.3467354143254171 0.7504608056350899 0.6222248346381599  
0.3427406638483365 0.5004689696439396 0.5395957950278545  
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0.1613229274159014 0.7504297128240810 0.5403324899856931  
0.6617675225558055 0.7504342579639338 0.4634448529006549  
0.1617072099946299 0.5004398730968798 0.4644674558654120  
0.3430737772117971 0.7504414246581047 0.4631677593626703  
0.1585691412592118 0.5004577839316887 0.6232859507573845  
0.3443484464417099 0.5006667870501328 0.3807926290909464  
0.6609721102288927 0.4998121526916297 0.3811829306007409  
0.8487174705145003 0.7504243137247733 0.3816986901851850  
0.8433042497998748 0.5005329182247893 0.4646052947230622  
0.8462796430033144 0.5003166022161184 0.6232959837193439  
0.6617616148998982 0.2504511509397074 0.4631627380132538  
0.8493341469130470 0.2502632216129623 0.3813983031589608  
0.6607872393721963 0.0013506599570959 0.3809018808560147  
0.3440459184860420 0.0003002580134219 0.3807698793276958  
0.3431107871094810 0.2504547273682892 0.4631454109159636  
0.1616057336995095 0.0004582833484961 0.4644013100663461  
0.8432919336930433 0.0004972456737538 0.4644773894304812  
0.1614191705216342 0.2504753509347245 0.5402900385639243  
0.8435232077672488 0.2504605021248036 0.5403370518964542  
0.6620646717884500 0.0004944005907664 0.5396126088282912  
0.6579950297685694 0.2503511178811200 0.6221025830932704  
0.3467640987514544 0.2504584731199165 0.6221224569809957  
0.1586162862197260 0.0004777408074825 0.6231424066513861  
0.8464121910035031 0.0005820521652991 0.6231878007878215  
0.1558147317193484 0.7502826444759699 0.3813655959124480  
0.1561857220721224 0.2505611572438414 0.3813289473863986  
0.3426892681732513 0.0004134682850214 0.5395399896096202  
0.7804836949045461 0.5731023699343112 0.2587433916046518  
0.7243521573448001 0.6830611818920900 0.2610655297043851

**N2 site 4**

1.0000000000000000  
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-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N

48 34

**Direct**

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0.3216408114509325 0.4993951067010558 0.6180456501184192  
0.1783861359544492 0.7491916214032165 0.6192487287969181  
0.8258443856558640 0.7488820390370622 0.6192387505333115  
0.1708660649313127 0.4993577752309910 0.5404489058774229  
0.8329899064860744 0.4985942858421737 0.5403263088422484  
0.6735714463253437 0.7483360283335528 0.5411923453392392  
0.3307826038537627 0.7489178792012013 0.5411822915373499  
0.0017785434949855 0.4993789080845572 0.4596619222890295  
0.5016396654289634 0.7488032056821494 0.4639187533133954  
0.5018435728860310 0.4985950936035697 0.3897325499799741  
0.0027610486055214 0.7507373425866828 0.3910660080287361  
0.3277779499400800 0.4999363933821387 0.4634519835478480  
0.1700257583233474 0.7505817435617872 0.4624761212493995  
0.8335922589098097 0.7498582303695496 0.4625752970701122  
0.1783662541165839 0.5006882814892615 0.3836526362906334  
0.8245684198122022 0.4989627567553850 0.3838437411997584  
0.6816702365700513 0.7494123145720752 0.3860227134539299  
0.3238419503379163 0.7506963069733397 0.3855994479095541  
0.5021371546103979 0.7499310017633987 0.6128735596824680  
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0.0021137063846370 -0.0005766723633157 0.6091570715562403  
0.6819315872069716 0.2487605478644108 0.3863584649665770  
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0.5019579706808137 -0.0009445414188173 0.5412977913844517  
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0.6843408681077874 -0.0010920210251273 0.6175020620174886  
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0.8324016105597996 -0.0010652188163833 0.5401831577663084  
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0.0017438019565607 -0.0008773545208708 0.4605562308218720  
0.8199922347276237 -0.0008121713256057 0.3847946935887135  
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0.1827752420355037 -0.0003561612295663 0.3847623751852987  
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0.6721664279555359 -0.0012101277584785 0.4635681569315193  
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0.3447183410747051 0.7501977607266662 0.6226697529323574  
0.3424685110660308 0.4994310726698791 0.5403012121851807  
0.6613418811973809 0.4988010587208018 0.5403576132807948  
0.1611253429088107 0.7492395872863112 0.5392494840386708  
0.6616225274241134 0.7486884108704047 0.4642135999301200

0.1601047201194114 0.4995586155648036 0.4633061004000636  
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0.3439187754839780 0.4978299807766936 0.3816408150511305  
0.6593210676533910 0.4985772947235640 0.3820762192907424  
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0.8457670199296443 0.2475946539162040 0.3802751613636430  
0.6548862932325006 0.9991239153161422 0.3827587614885802  
0.3481563591971528 0.0026720777170325 0.3826464914170685  
0.3420231612499469 0.2500725727227363 0.4639052553966989  
0.1603102811804600 -0.0005719994619974 0.4631823444516686  
0.8432036886355696 -0.0014639377544612 0.4631001270805198  
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0.8427812767664006 0.2489940146980170 0.5391579040690834  
0.6618380754432972 -0.0012553846041915 0.5404929257099593  
0.6590438461704580 0.2479272201530996 0.6224778244445819  
0.3451799407361623 0.2482611926727607 0.6223916211095718  
0.1562843559653886 0.9996979504316855 0.6222961177641270  
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0.1582619676092621 0.7516907698308134 0.3803516751620654  
0.1562023039796540 0.2486575259664851 0.3802088000144370  
0.3421661875575858 -0.0007504047533499 0.5405165390173525  
0.4662077955667155 0.2734164633518023 0.2678110952381852  
0.5523446218685149 0.2722171402955086 0.2838656803288558

**N2 site 5**

1.0000000000000000  
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-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N

48 34

Direct

0.5021542838082848 0.4994382411276582 0.5388880229240479  
0.0021895195395697 0.7503511111772696 0.5408141536244006  
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0.3233048993418186 0.4984746993156297 0.6176774723945042  
0.1787984621911768 0.7480574920815021 0.6176799238398671  
0.8254692597233553 0.7523556983426719 0.6177336034802311  
0.1713813691261236 0.4974380819041215 0.5391682488265904  
0.8325362704211319 0.5033143025499338 0.5391054143953087  
0.6730262689187652 0.7535759054531934 0.5396329603762263  
0.3313551973345344 0.7468772861439261 0.5395059752308660  
0.0015620176728195 0.5010771916009685 0.4595250611287895  
0.5022449713102872 0.7536526037847001 0.4654459545866104  
0.4975387203828934 0.4967150563161202 0.3779329436077336  
0.0021402878910437 0.7500886761203998 0.3933010409388992  
0.3324298457224781 0.4964473772751428 0.4603689576264504  
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0.1714540300633400 0.4947245347671902 0.3832769959938062  
0.8256474867154295 0.5082536988500265 0.3829957491760649  
0.6789834164560209 0.7630486869038275 0.3773144164899886  
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0.6903715353745332 0.2587440635992000 0.3845810273825396  
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0.6814685717426442 0.0022558052297098 0.6175333252781043  
0.3227264797037481 0.9977037009713128 0.6173930479473321  
0.1820993747301319 0.2479743076933685 0.6164313433639357  
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0.1728359303964316 0.2455476927816961 0.4616511716006686  
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0.5065376864007303 -0.0002482743127872 0.3822822863624336  
0.5021595030672574 0.2471959559919743 0.4619728760198254  
0.6728389132095645 0.0043042248730252 0.4604996202716526  
0.8426161059573349 0.7531399335876769 0.5375791299033233  
0.6593766800390354 0.7527972664230370 0.6206586986715589  
0.3448905301790912 0.7482015874633913 0.6205743719733974  
0.3426406574949524 0.4972072318583237 0.5379292821834349  
0.6616826309030922 0.5035023535424004 0.5377868947307888  
0.1617531358920004 0.7475704262450472 0.5374992381134007  
0.6610221075676498 0.7550714577622195 0.4610555507940407  
0.1615164404492810 0.4962430180187457 0.4625562389534745  
0.3435055670529044 0.7454375457308448 0.4609288342533782  
0.1577074993148458 0.4967239206037667 0.6210649958909604  
0.3352294273244223 0.4816114990381344 0.3819943257962585  
0.6611387435733849 0.5027928877841056 0.3796550097873782  
0.8490307957971498 0.7554408922212442 0.3791698945761861  
0.8416982382195831 0.5044251298909225 0.4622534141586521  
0.8467716050472601 0.5015795890770769 0.6211474039643226  
0.6609342590399452 0.2556552347645054 0.4613471904738956  
0.8507692659810078 0.2589029215968318 0.3789505023594872  
0.6687945380708484 0.0184786780763053 0.3825768069683709  
0.3436482837866273 0.9973771822810644 0.3800122272785559  
0.3433132591531488 0.2446908770351406 0.4612224450847429  
0.1623007457970419 0.9962873357546652 0.4620773145436984

0.8430635686098698 0.0044811472332285 0.4626421217055990  
0.1611048768460820 0.2473008594133350 0.5382739050419930  
0.8431705674149762 0.2532198403793113 0.5383445465831296  
0.6616205803421218 0.0034537668436408 0.5382780529525054  
0.6579801131343240 0.2526912157940978 0.6205526109055352  
0.3462716873944784 0.2476837364197929 0.6204339558006170  
0.1575827521282048 0.9990875571985128 0.6210215298309072  
0.8466086222522214 0.0039083596902050 0.6211558870620958  
0.1551765984395350 0.7454028556953645 0.3791429572562030  
0.1534928271179079 0.2412623765438548 0.3789354279161983  
0.3427657973997650 0.9972335996036837 0.5379393071502054  
0.5395978331872197 0.8071017576146848 0.3375498721142086  
0.4640411858634116 0.6983699283194530 0.3368412336078382

**HN=NH site 2**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 2

**Direct**

0.5025513135886730 0.5006689929007030 0.5394889965463540  
0.0031075571431648 0.7503141047341458 0.5403350753530741  
0.6819389805002651 0.5001486170240468 0.6167307017532793  
0.3242419519532611 0.4995853098430959 0.6173843637618435  
0.1826592276155750 0.7496015440474172 0.6172423320808004  
0.8232918603632385 0.7506234125195147 0.6167661690755121  
0.1719955134276736 0.5000204127793325 0.5399253882275725  
0.8340781425271709 0.5005766867248174 0.5390129855906733  
0.6741987768614356 0.7505359704598837 0.538748855529495  
0.3316570102308228 0.7499761662440748 0.5392515980932081  
0.0029233592706354 0.5015586202391442 0.4598997713656336  
0.5023612055415803 0.7518806366399370 0.4611833256148050  
0.5008128909361941 0.5017059820668908 0.3877221084060729  
0.0021355783456641 0.7500752648572521 0.3922104631840234  
0.3315244122581332 0.4989783459322216 0.4609532260285574  
0.1730723598414573 0.7497918761222827 0.4618667326146939  
0.8321032193619952 0.7493636412915644 0.4615688788480244  
0.1773960240536905 0.5004482256665036 0.3829670909337042  
0.8264373294383728 0.4954146579707123 0.3787511930494926  
0.6870747921063470 0.7507660031710938 0.3847891179421200  
0.3183719508424409 0.7500460819110192 0.3847827937620524  
0.5028599579749186 0.7504628558420241 0.6091508335525390  
0.0029552049430810 0.5004121399654881 0.6101624212044588  
0.0028017419169281 -0.0004221756720389 0.6103489669192648  
0.6858891588231601 0.2535184640005954 0.3792649524526588  
0.3207573299188561 0.2489548720371289 0.3845734795676635  
0.5027956732101914 0.2498097528365517 0.6093498925318488  
0.5025792978559718 -0.0000866001538688 0.5390042663936284  
0.0030373470073357 0.2493466171032747 0.5405361479899853  
0.6815527527648650 0.9998861442390761 0.6167448723109525  
0.3235875148934433 0.0003012749243247 0.6169832615567119

0.1814260121412785 0.2501123721944123 0.6177401196142125  
0.8244121080259410 0.2500106048202388 0.6169664792985607  
0.1726865986555683 -0.0003250069232760 0.5399266364348484  
0.8330502067037823 0.9997329264840464 0.5392678560865296  
0.6729524088442510 0.2497863892096685 0.5384840900827139  
0.6744119689363506 0.4982294560527738 0.4614624392960024  
0.0034000001677957 -0.0019991561137079 0.4610526975209767  
0.8265580505972341 -0.0000355103933388 0.3831688991494839  
0.3317235363007786 0.2500547364061746 0.5390920966203769  
0.1793959720431024 -0.0003298975209213 0.3830156121322640  
0.1709920541474456 0.2498956719365766 0.4619958737539066  
0.3317741987348491 0.0005320526989321 0.4611155926390194  
0.8356966357907706 0.2513849782423202 0.4624717664887015  
0.0054578469998593 0.2485482472753569 0.3967661603431328  
0.5033935640354222 0.9986063967228694 0.3871998076117794  
0.5034238436669350 0.2487484073261892 0.4599633657037990  
0.6745162219172295 0.0018439815658393 0.4607245423256527  
0.8440321536440292 0.7494702729189896 0.5382466597915292  
0.6585425434611906 0.7500444739865990 0.6204879162952968  
0.3471870584208297 0.7502644142848891 0.6206071760586808  
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0.1620045158195300 0.7498349875253543 0.5387356987956725  
0.6616994517387094 0.7506794237403265 0.4616544107387385  
0.1622576839178550 0.5001730299288677 0.4630274682979322  
0.3431146243671605 0.7499022833935358 0.4617365678291497  
0.1588640165018358 0.5002717169488758 0.6218246022966638  
0.3425271167323744 0.5009423569692670 0.3791829476551554  
0.6583246249276027 0.5059344930082346 0.3850355323976837  
0.8486663802412052 0.7501913826397635 0.3797020875359013  
0.8435584630818059 0.5013475397366782 0.4588574191770018  
0.8468459568311658 0.5005294056486976 0.6202509450080411  
0.6627728698784473 0.2493410581597320 0.4579447506282068  
0.8533905579890595 0.2461850608427415 0.3856105587478881  
0.6613781422375357 0.9992166268923943 0.3794812379307196  
0.3451077394404660 0.9986184532229977 0.3791504049246900  
0.3437693928499305 0.2499431276920490 0.4616455730537299  
0.1625285374742716 -0.0005856539326578 0.4630929109862147  
0.8439541163031595 -0.0005399722792532 0.4627897925889796  
0.1620907158154681 0.2497892755174635 0.5387372049508571  
0.8435723725003540 0.2505428646463438 0.5387244791538267  
0.6623103348173640 0.0007009158520773 0.5376446057474050  
0.6590615985043068 0.2502483051476044 0.6193587391307794  
0.3468175496707069 0.2496302874713387 0.6206848650752570  
0.1587265680115381 -0.0005999311646411 0.6216133486066554  
0.8468644054329403 -0.0001090396166791 0.6214488089971099  
0.1561364097267677 0.7505638404968930 0.3794261251144966  
0.1570054643610023 0.2493888652320458 0.3803225615505179  
0.3431448101219617 -0.0000482975405993 0.5381650683258266  
0.7203375096792566 0.3112726993299321 0.3060743838412944  
0.7929827139374731 0.4340912365599741 0.3058912645692498  
0.6974539526293949 0.2682315865174713 0.2705129168323446

0.8173710132331838 0.4741299121109451 0.2701594162112368

**HN=NH site 3**

1.0000000000000000

12.0322999999999993 0.0000000000000000 0.0000000000000000

-0.0000000007000000 8.0876000000000001 0.0000000000000000

-0.000000022000000 -0.000000022000000 26.0656999999999996

Mn N H

48 34 2

**Direct**

0.5021206797468438 0.4998069541573967 0.5400248233396803

0.0026178634693705 0.7511242023993766 0.5410684541981056

0.6816191676392824 0.5003223107329426 0.6172345482716602

0.3237481739466185 0.5008699092063587 0.6178778299176400

0.1809302376883524 0.7503586112884372 0.6183118972017178

0.8241145423666482 0.7504844188000637 0.6175096492113195

0.1715537400241936 0.5004267228405858 0.5404683795725768

0.8336736197450947 0.4999301312619386 0.5395241885570160

0.6725273881171816 0.7506996512937083 0.5390441705732605

0.3312877544196693 0.7504222370035903 0.5396499282208783

0.0024116469715054 0.4988762247880238 0.4604075937122414

0.5028932270334645 0.7517436682680367 0.4605412247286396

0.5002183934802549 0.4988186260308796 0.3882808009818087

0.0047976917973854 0.7519214389913408 0.3972774562044274

0.3309764056064479 0.5015002311638179 0.4615144080860942

0.1703889683307736 0.7505680394142363 0.4625368494822832

0.8352478106462154 0.7491415956631390 0.4629695468655300

0.1768646595237766 0.5000234581028515 0.3835083849550422

0.8257468486680570 0.5051350882640079 0.3792002409752624

0.6852653049100670 0.7470533583754446 0.3798215715619099

0.3201895728026662 0.7515428663119216 0.3851055673610667

0.5024370178201953 0.7506255650689424 0.6099541900934926

0.0025750568391552 0.5000333985762254 0.6106360411248901

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0.6864574984101768 0.2497471975680297 0.3853376773295340

0.3178788105864477 0.2503835196509108 0.3853145874829335

0.5024755877695596 0.2500238554323804 0.6097471233099793

0.5021481522215860 0.0005456088284722 0.5395574673721373

0.0026896331271238 0.2501437240476254 0.5408646723399433

0.6812289580829798 0.0006022539661126 0.6172567186483053

0.3230992285756273 0.0001555473498951 0.6174933085007870

0.1821877089666015 0.2508338510683851 0.6178037420315816

0.8229863511423677 0.2498389834505403 0.6173104745425205

0.1722529230052870 0.0007930984097599 0.5404742666210314

0.8326423376336574 0.0007465057316264 0.5397762236813043

0.6737607043893928 0.2499441254169315 0.5393191352400402

0.6739309357542526 0.5022494382877993 0.4620463363072418

0.0028914366728011 0.0025026418687327 0.4615781237378087

0.8259389822227455 0.0005335441051397 0.3836713284361751

0.3312194880960434 0.2504726973617442 0.5397975355250197

0.1787928397149220 0.0008081704287709 0.3835445846875820

0.1725374711381006 0.2506769120586886 0.4624080395935401

0.3312437563259666 0.9999347771999049 0.4616664770939891



0.8315914974352070 0.2511481417842228 0.4620886681367585  
0.0015339608413483 0.2504267022766116 0.3927122799729758  
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0.5018387434580139 0.2485735174582157 0.4617578480195053  
0.6740180108541706 -0.0013317519151263 0.4612878806647896  
0.8431576952515107 0.7498977935328182 0.5392554049192654  
0.6587721046800874 0.7502169991836104 0.6199123245143033  
0.3463578485267869 0.7507889066713541 0.6212272300553722  
0.3424389763573227 0.5002436771832306 0.5385414392300865  
0.6619016236422465 0.5006119823717570 0.5385808481059421  
0.1616396318980212 0.7506434922610037 0.5392734633783236  
0.6622876771161306 0.7511219820538859 0.4585102259108508  
0.1617113710908339 0.5002878873508403 0.4635453568485439  
0.3432259915650984 0.7505323683555133 0.4621727216907736  
0.1584049691801570 0.5001876112040979 0.6223441999400985  
0.3419503377357244 0.4995302178680147 0.3797481017769998  
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0.8527831224953559 0.7542691015742591 0.3860840883435585  
0.8430463452536201 0.4991981781573271 0.4593876406649174  
0.8465467294688895 0.4999497931811374 0.6207822414382178  
0.6611962322663850 0.2498727165176118 0.4622115258384608  
0.8480609560749608 0.2503780390774661 0.3801951722618048  
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0.3445332437399477 0.0018322725033561 0.3797088029075485  
0.3425764101635275 0.2505409429620242 0.4622705965045956  
0.1619985677852655 0.0010212810507245 0.4636147166168971  
0.8434666809349950 0.0009899505882332 0.4633115827710191  
0.1615624570564809 0.2506218090959159 0.5392548049954345  
0.8436385125910580 0.2510405111821116 0.5387551758843842  
0.6619316989126245 0.9997705203977756 0.5381873023590500  
0.6582340202618117 0.2504764298434050 0.6210341547705092  
0.3467505556386655 0.2501982482981903 0.6211472380529277  
0.1582625557209442 0.0010487461188883 0.6221362045293368  
0.8465492782910263 0.0005763501281761 0.6219777577546043  
0.1565097717400811 0.7510607884809967 0.3808414867460361  
0.1555968551120029 0.2499174062258999 0.3799420226653897  
0.3426806263521825 0.0004976009468413 0.5386922684688739  
0.7917149695463864 0.5664132795748628 0.3063183368229822  
0.7191165946649344 0.6892801704461645 0.3066364104953798  
0.6952751016269854 0.7315505536387393 0.2712111641421494  
0.8148742130299934 0.5252992313775758 0.2706057247639003

**HN=NH site 4**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.000000022000000 -0.000000022000000 26.0656999999999996

Mn N H  
48 34 2

**Direct**

0.5020131896725810 0.5012185980053934 0.5398937732662428  
0.0020229795132360 0.7511693079843339 0.5416279035964051  
0.6826838886711025 0.5002463606777056 0.6174015608283602

0.3213678404874774 0.5000935606620025 0.6173897020769962  
0.1826042932555197 0.7514033165267252 0.6174262471568084  
0.8214213439800492 0.7515704422676217 0.6174672065203264  
0.1727964557611029 0.5001999337678694 0.5397608519015339  
0.8312148434114993 0.5003642047849830 0.5397852332038944  
0.6736008814158003 0.7510774191450081 0.5401860498440337  
0.3304358944430258 0.7508805901881135 0.5401654617063997  
0.0020622720024988 0.4995627663830657 0.4607858538281963  
0.5020590210383878 0.7498434752014305 0.4643521493974462  
0.5020927104258306 0.5146808782964387 0.3886072770725904  
0.0020628541772093 0.7516541723950012 0.3938559000417708  
0.3295987007293813 0.4995905143994981 0.4619196428977838  
0.1717545536969501 0.7524053620673464 0.4627526705419563  
0.8323881885572675 0.7526480827574369 0.4627788335286944  
0.1796573072213320 0.4998427269258083 0.3852941703691067  
0.8244849632838664 0.5000943090718322 0.3853466516551551  
0.6903086881210820 0.7516337626889990 0.3856921862458367  
0.3139189587602768 0.7512949074010598 0.3856559477878193  
0.5020038888166739 0.7497787409221580 0.6096859816518828  
0.0020133504922881 0.5013940032173732 0.6103709050073596  
0.0020148425838891 -0.0002985558801120 0.6116721674635749  
0.6759995541960889 0.2516869696819768 0.3786484681085467  
0.3279005875868218 0.2515073918314910 0.3787159729652385  
0.5020040442496627 0.2515179153345658 0.6107441475169919  
0.5020205325382592 0.0007446512300868 0.5401597275378622  
0.0020137874485323 0.2505111451604333 0.5417844372533724  
0.6788400096326330 0.0009473361072809 0.6193086946493184  
0.3251555542570703 0.0008117751184453 0.6192812749297125  
0.1793308288506141 0.2497818598951534 0.6184346259310923  
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0.8322632967320172 0.0014259548738513 0.5402496450259450  
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0.6745522707498378 0.4998446324043342 0.4619603820716159  
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0.8293312889819183 0.0038264808541767 0.3840407866577988  
0.3328003970769330 0.2508713814296724 0.5399102481187003  
0.1747970903632843 0.0035718302965418 0.3839784867654258  
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0.5020532990808426 0.2509835876156450 0.4613921173869489  
0.6683569376789708 0.0027139803884229 0.4609595838353603  
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0.3429838400685653 0.7509361560207176 0.4624758744630159  
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0.6619102020864064 0.2516705261696345 0.4612400376367896  
0.8476567493753302 0.2525179148267476 0.3797858418523585  
0.6642124224369207 0.9890250754219174 0.3828758027525668  
0.3399881495670107 0.9886486979194095 0.3829011635016493  
0.3421908806177809 0.2514089907995022 0.4611955474200697  
0.1621238849613358 0.0008121278884024 0.4635833380645579  
0.8420017989388046 0.0010206489490263 0.4636080546957007  
0.1615783483825136 0.2507849567276845 0.5384365632956173  
0.8424527287829855 0.2509534805487839 0.5384573925052770  
0.6615057012288287 0.0012946644275173 0.5383855823537601  
0.6585833959904777 0.2521748372377938 0.6213092845147522  
0.3454280131807662 0.2520042962995572 0.6212808086404736  
0.1583420371003611 -0.0004002955421879 0.6221368615566869  
0.8456901830820881 -0.0002475520227409 0.6221655431769575  
0.1535384158972016 0.7476321997618395 0.3798943505703272  
0.1563577532403490 0.2523027207364633 0.3797665250632732  
0.3425443434705546 0.0011209850942534 0.5383681772559963  
0.4438642511832694 0.1924541334713494 0.3191786848914978  
0.5597269489571821 0.1945642182045935 0.3189398267483931  
0.5903053144754833 0.1245619321641879 0.2890281932324229  
0.4136565329847420 0.1215167208635987 0.2893916094698883

**HN=NH site 5**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 2

**Direct**

0.5020804030213493 0.4995828086105212 0.5390953024200007  
0.0021693035494170 0.7502779768533527 0.5410360532063658  
0.6805659158959182 0.5026128660024640 0.6181137820580482  
0.3233408215865470 0.4985109371919487 0.6178471889941399  
0.1794798750322672 0.7483106679806472 0.6173964056736038  
0.8245791920670695 0.7522017930317195 0.6175479063492479  
0.1716320765405017 0.4975430884424579 0.5393656658907632  
0.8321120952185439 0.5033800184966842 0.5393736831289858  
0.6725265310206652 0.7534489294553646 0.5396166392372039  
0.3318065604896934 0.7471288277349070 0.5394707873979531  
0.0016317202837392 0.5016128435078188 0.4602463836447146  
0.5022662332382580 0.7527465467742090 0.4640684910059885  
0.4981826692124835 0.4944721508813287 0.3789200139926063  
0.0020693799585443 0.7501329190144860 0.3926174300086910  
0.3323096520914258 0.4961598419931600 0.4603375214426432

0.1738077936959236 0.7460947596782553 0.4610903032395082  
0.8305584432844025 0.7541072406529996 0.4612216473742898  
0.1710450782953611 0.4937178555189690 0.3837415890342425  
0.8256519713301861 0.5089918397421980 0.3837202681956702  
0.6809314785290017 0.7639310410126484 0.3779000954407410  
0.3227833790186396 0.7390588459629560 0.3771116861334285  
0.5020597570615476 0.7503904370002970 0.6102956949369261  
0.0021040259494329 0.4993223988026563 0.6103076508330345  
0.0021031932014588 0.0013569034420589 0.6103078168948558  
0.6902210902641658 0.2591836805458942 0.3850933166262825  
0.3144386544381859 0.2394575751529496 0.3847249037744065  
0.5020594606042412 0.2503370124623390 0.6091410717965651  
0.5021610209939568 0.0009317144198335 0.5393639748642401  
0.0021193569708783 0.2503252582965792 0.5407221335892305  
0.6811094188258596 0.0021998116470703 0.6178207222777407  
0.3232676442751907 -0.0018811961745139 0.6177985967991712  
0.1823262986197847 0.2480699997021870 0.6164696108780140  
0.8218164201031650 0.2527935488406641 0.6166555874281047  
0.1725132382782278 -0.0028045874921520 0.5391614475089637  
0.8322622711743952 0.0030571625791509 0.5395082031836845  
0.6732540762381721 0.2535423500245022 0.5395270241836374  
0.6699309479287036 0.5070098828943088 0.4601123294409564  
0.0026458145227383 -0.0009310333327599 0.4604678778281056  
0.8333798052205604 0.0066343779083859 0.3840019525503069  
0.3310578409886595 0.2471644584572227 0.5393572749820643  
0.1787371962902339 -0.0083688742550542 0.3839148764619015  
0.1725587003953702 0.2452916283268665 0.4620018730873158  
0.3338821877419694 0.9935067082402753 0.4598697855892767  
0.8318133249074036 0.2555909311896375 0.4621494812768486  
0.0021706636641722 0.2506027664454975 0.3934504754366956  
0.5062947152075850 0.0026862311335960 0.3830810717164777  
0.5021742701541108 0.2473563058846261 0.4618261183903328  
0.6726496209583286 0.0045908355251447 0.4604890352202687  
0.8428026848643297 0.7532092970452084 0.5378933230454248  
0.6589006849791806 0.7527100023496671 0.6207074767922438  
0.3451809895302571 0.7481654222910881 0.6205152890586476  
0.3426034814157827 0.4973307972467960 0.5377898112719682  
0.6615088239102458 0.5033864238810355 0.5377668636284150  
0.1615120257776647 0.7475136204651385 0.5377428060920599  
0.6609276131415996 0.7551273870992417 0.4611995980675257  
0.1616038845580536 0.4961723565376586 0.4627512192959911  
0.3436575264795518 0.7452453337808669 0.4609370649339099  
0.1577682332603963 0.4970916185581776 0.6212054608477899  
0.3351943145959252 0.4811270092664910 0.3812601656601928  
0.6611325299744257 0.5045063519782429 0.3793758413235685  
0.8484451882870995 0.7553561884886445 0.3795984205708346  
0.8418471309771599 0.5046574618867229 0.4624923912580812  
0.8464487923774109 0.5016112357270612 0.6212769749541432  
0.6609798618433221 0.2557947396267659 0.4615606519414386  
0.8507914782795456 0.2598581254716937 0.3792745443858373  
0.6689740575605966 0.0190361009974343 0.3818459410555659  
0.3436818489877290 -0.0045298470569707 0.3795188033905679

0.3432991729196258 0.2445377293921010 0.4613675269685192  
0.1623599180757378 -0.0039912716140130 0.4622524675347711  
0.8429734250503488 0.0045298717815823 0.4629058608452615  
0.1611026701260285 0.2474363064499691 0.5385023402867107  
0.8431885702340556 0.2531669787390690 0.5386498407165561  
0.6615629128999404 0.0032599578580650 0.5381252664562548  
0.6577513189831625 0.2523950443405815 0.6207225966983997  
0.3463674794726303 0.2481118397345951 0.6206002950518488  
0.1577574107360030 -0.0009059522829986 0.6211160865018552  
0.8464062066222017 0.0035656259009329 0.6213237081773885  
0.1556007465462904 0.7455462425909564 0.3794490827802948  
0.1536335779535946 0.2403759168104901 0.3792119949684861  
0.3428327605223912 -0.0028183988036557 0.5377547161303723  
0.5438159683759660 0.8153374727011250 0.3322768992527126  
0.4601804037633332 0.6909211519080657 0.3309452000457027  
0.4418868068318830 0.6565747021149156 0.2939060104813832  
0.5632189765897059 0.8566913636173800 0.2960661936895149

**N=NH site 1**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 1

**Direct**

0.5027395442048568 0.5024728126619599 0.5391397252605220  
0.0030646544048869 0.7518754053198201 0.5408712798035971  
0.6801960900995939 0.5023246413393925 0.6180272437722842  
0.3254329683951657 0.5020384469181625 0.6176924031657957  
0.1831668143024277 0.7519744722175021 0.6166793713337357  
0.8226432944227319 0.7517088551857926 0.6172831942913026  
0.1721007413947687 0.5024923467525826 0.5396092037590552  
0.8337736035346404 0.5020780192662263 0.5396401765855493  
0.6748771931500337 0.7518864243095522 0.5396255812482831  
0.3314002449294877 0.7523174408923311 0.5390054741041309  
0.0033038625272692 0.5026097154821292 0.4593528424383600  
0.5028516240083484 0.7530419151954117 0.4629064118445280  
0.5028388781124110 0.4876592902291903 0.3752364167795986  
0.0030735804914110 0.7513661296828045 0.3927110344021191  
0.3343498780915361 0.5017295077265504 0.4603404916803074  
0.1730910517850688 0.7517172251267320 0.4616528394285744  
0.8332326773622802 0.7505322046939169 0.4621224957003657  
0.1764025595328387 0.5028895653745004 0.3822749754036851  
0.8283386553676720 0.4997572094449740 0.3827848257494533  
0.6902554397709847 0.7519180335602600 0.3856275242818835  
0.3176955372349503 0.7525612258588318 0.3843925744567038  
0.5028393755564052 0.7532248435025017 0.6088595753539385  
0.0029332313253930 0.5029365146499172 0.6110030409857741  
0.0029995698532634 0.0016823769823027 0.6100835547307589  
0.6816536213856943 0.2510037567854534 0.3801719149579283  
0.3215879955447076 0.2536033027716347 0.3829191031870334  
0.5027715049495988 0.2516340488896200 0.6095850870976135

0.5026054180957509 0.0023000215996382 0.5392825894012732  
0.0030928342197253 0.2528461384832188 0.5412874071417803  
0.6834758475014594 0.0022088312453864 0.6165927317376816  
0.3228717380528546 0.0027220429367566 0.6166016475120056  
0.1808734730111563 0.2528945084905266 0.6174206895559984  
0.8253828801377755 0.2527256011643542 0.6176616230391521  
0.1728584566478767 0.0024971290286056 0.5393323969509611  
0.8327189948041566 0.0021387220870111 0.5394387361164262  
0.6731561991044240 0.2521821172965475 0.5390865077971332  
0.6719278072392366 0.5007432177982746 0.4610608947808574  
0.0034546725001100 0.0019542443860027 0.4602420011993429  
0.8262659841505345 0.0021948596190879 0.3842434367502478  
0.3319912135251163 0.2526129428306556 0.5387026689407407  
0.1805980492323100 0.0026249773201508 0.3835207428854140  
0.1709536759491746 0.2532970872748059 0.4613859778172342  
0.3313286157853066 0.0034960555492774 0.4607738518250749  
0.8359421481554382 0.2525675984477331 0.4617174186191254  
0.0027967410126065 0.2497407052915931 0.3934291031458461  
0.5032466716132334 0.9950933816374261 0.3880655344417651  
0.5040166140434402 0.2522764306310508 0.4601476951270006  
0.6757743298045611 0.0028069485108718 0.4615503744909054  
0.8442085843683829 0.7522765876311028 0.5387470935917908  
0.6583028223360577 0.7532238738752082 0.6209034990396746  
0.3473357920106078 0.7531614339110141 0.6202637795083549  
0.3432410459833909 0.5022679020207141 0.5376996871010433  
0.6625934399889359 0.5018036936032670 0.5382051484354167  
0.1619338650610842 0.7525670225679592 0.5384157888525214  
0.6621327917969652 0.7517732769814202 0.4621688316584442  
0.1627802834503609 0.5025913824795845 0.4628522998828837  
0.3436586399802648 0.7522455058816790 0.4612836334369298  
0.1591733424433079 0.5032006557061547 0.6214474013949718  
0.3426746372977100 0.5071650148378619 0.3804922071677423  
0.6627161605319095 0.5104473037001178 0.3838175965459278  
0.8507824343234875 0.7532708988591709 0.3793823088918788  
0.8436574960810820 0.5017330734063739 0.4630759557254145  
0.8465545704546418 0.5029081352727393 0.6216337143626617  
0.6642405123897607 0.2517377406971042 0.4594255376293536  
0.8493508679798362 0.2506710168727118 0.3796510811550152  
0.6623912738571255 -0.0029233390808358 0.3814267010479807  
0.3452258079538119 0.0015733612904916 0.3789787814630858  
0.3440089816050458 0.2527126929145234 0.4610494559649003  
0.1624889730240498 0.0021081481423002 0.4623511070288154  
0.8444688305344726 0.0010392824622956 0.4625994864963977  
0.1621528487873842 0.2523892197960684 0.5382710159179085  
0.8438703726394523 0.2518792050263295 0.5382799083659565  
0.6620393762489012 0.0024665617841159 0.5384547478336210  
0.6593738593152177 0.2509422471990425 0.6197521890993780  
0.3464755987548572 0.2514425854557817 0.6203628163635695  
0.1585425360797325 0.0016022055688719 0.6212705465369913  
0.8473784896363672 0.0012461995414492 0.6214026069475207  
0.1558957120980125 0.7551827088587255 0.3791008287336348  
0.1562548525035593 0.2520426530156227 0.3795815871845051

0.3433337786002864 0.0024009844141852 0.5379325741847616  
0.5267945491929743 0.3737504058119900 0.3156117431291871  
0.6115817598739445 0.2779196687933146 0.3127259567080378  
0.6191147245017159 0.2112809465761064 0.2792361157901069

**N=NH site 2**

1.00000000000000  
12.032299999999993 0.000000000000000 0.000000000000000  
-0.0000000007000000 8.087600000000001 0.000000000000000  
-0.0000000022000000 -0.0000000022000000 26.065699999999996

Mn N H

48 34 1

**Direct**

0.5022362201630647 0.5002170454662236 0.5399042088442273  
0.0026454792319631 0.7502337133569216 0.5402566514812920  
0.6807201549639098 0.5001845906527297 0.6171410760074731  
0.3235936440037652 0.4993891649239470 0.6176676038555776  
0.1828463633768677 0.7498026885590833 0.6170618747452242  
0.8217924917244579 0.7501450256692369 0.6164999626684435  
0.1716669437412973 0.5000534217843439 0.5399152485618799  
0.8332837302237255 0.4997915539892542 0.5389135514000377  
0.6731258114013506 0.7497129220236012 0.5386994729100649  
0.3315307208259473 0.7499535363753799 0.5393717369137766  
0.0028344966281345 0.5005754836816741 0.4598656257252601  
0.5026445665326603 0.7515411043127134 0.4614658668512700  
0.5013211030163499 0.4984170472699962 0.3878680318296482  
0.0023059665627752 0.7500238580392170 0.3918687840162439  
0.3313698544372030 0.4990919375227723 0.4611602055977893  
0.1731098348293622 0.7498363280106228 0.4617342469021590  
0.8312664800571208 0.7489413821405366 0.4612422711810153  
0.1781882795785711 0.5006959915441649 0.3828246136822407  
0.8281333829500848 0.4985275729086399 0.3790251772203020  
0.6831689397356435 0.7501234293267749 0.3829373789961417  
0.3196467480352119 0.7502298735973810 0.3845481476078156  
0.5022556210809562 0.7504804227744628 0.6091674209849863  
0.0024340879569357 0.5006865545454517 0.6101480797242103  
0.0022957104541076 -0.0010544522221388 0.6102937644383506  
0.6935971569103987 0.2555310331703870 0.3741039054544417  
0.3214835013445126 0.2495277270534186 0.3842345813526266  
0.5023184418062249 0.2495803237539989 0.6100916482993967  
0.5020160555033892 -0.0003115538947658 0.5394166761998901  
0.0023499832778905 0.2491483202077515 0.5408460121058078  
0.6817819632208565 0.9995145781822378 0.6166500996925635  
0.3232208342766465 0.0004391899005530 0.6174660572265968  
0.1799310141702282 0.2499636584391322 0.6180510549361451  
0.8249619069639401 0.2496054137815338 0.6174571371998717  
0.1721891282228356 -0.0001542472661040 0.5399051895960658  
0.8318877166326134 -0.0003750255679069 0.5390016034475762  
0.6717966405334800 0.2494755569743983 0.5391577568035243  
0.6738725774921486 0.4970704759696217 0.4609483188667823  
0.0033652280372307 -0.0020223106287282 0.4608438783471337  
0.8263730562778641 -0.0014169542628176 0.3833349122993401  
0.3312037571786435 0.2501917493476317 0.5392700245024078

0.1805787973114026 -0.0003553065970772 0.3829376333193835  
0.1705806090722138 0.2498000132376297 0.4619198451205254  
0.3318755687380921 0.0005370529146422 0.4612153039413535  
0.8345335657439560 0.2508478008886429 0.4622194260762313  
0.0059615813885289 0.2489146219370901 0.3945888367982741  
0.5043291757475907 0.0028764671192534 0.3878569634046977  
0.5032661218927975 0.2491893659024870 0.4605298450823083  
0.6741495252218269 0.0026003952514864 0.4606351634937527  
0.8432957116869475 0.7490303504335983 0.5381405687378867  
0.6575758714462768 0.7501714905561481 0.6207449941964289  
0.3469387504446197 0.7501537275056244 0.6208169565350808  
0.3426867909004986 0.5001555127196502 0.5382540884875258  
0.6618835058040373 0.4994946844088169 0.5380493452326153  
0.1616159851011556 0.7498504731992897 0.5386986028603503  
0.6617370940510402 0.7502658700750034 0.4615274009834892  
0.1620066570652998 0.5000681111458010 0.4628675458173236  
0.3434668759080155 0.7499190157322393 0.4618284531178614  
0.1582468418282336 0.5009733199817967 0.6216839126255678  
0.3433966230818846 0.5008735503916827 0.3794005395197410  
0.6589985384433742 0.4998109828963862 0.3844449182675111  
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0.8461816186303348 0.5008589010707527 0.6199454770402320  
0.6624519874460006 0.2492902430355809 0.4607138010797833  
0.8530415970937724 0.2447422930311206 0.3853628809647703  
0.6623538452654819 0.0037737410174730 0.3797130327613386  
0.3462427837947773 0.9991274924364051 0.3795671184820970  
0.3433744664417623 0.2499564644303371 0.4619141270855033  
0.1624717623616461 -0.0006004683287092 0.4629414006281716  
0.8436969415427840 -0.0006551670155704 0.4623002080300882  
0.1613697897271800 0.2498786839385908 0.5386972362809761  
0.8426834943101119 0.2500149007183296 0.5387116263976192  
0.6616017748973857 0.0002223678309663 0.5380587023256576  
0.6591484285163804 0.2494681882331803 0.6197087679675577  
0.3459769379845525 0.2497302181096553 0.6209497368689429  
0.1580649297017378 -0.0011562421098252 0.6215917205548442  
0.8464634654015381 -0.0013795547383010 0.6211291092327249  
0.1567529228993327 0.7506523833616200 0.3795258470677939  
0.1578923225496814 0.2491550781503629 0.3801110764133092  
0.3427671809244028 -0.0000311879191310 0.5382771937451729  
0.7243232944087051 0.3119820880943743 0.3068512339360798  
0.7928229192156465 0.4325111750246494 0.3055365130368143  
0.8135617813473088 0.4743784687538570 0.2693491391486754

**N=NH site 3**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 1

**Direct**

0.5021017159281600 0.4998442576299989 0.5398794399771519



0.0022237506183418 0.7512301571828580 0.5413322700307019  
0.6806128878227098 0.5004120875003227 0.6172569660706272  
0.3241034662963642 0.5007772446040430 0.6179396602651231  
0.1803964890938926 0.7501443231075489 0.6182796801152250  
0.8242029505686609 0.7508355748390314 0.6178588703544161  
0.1714027296513274 0.5004467558122087 0.5402469875157172  
0.8335331038233731 0.5002772539563189 0.5400497900538852  
0.6725453749141391 0.7506207130866807 0.5388516567070445  
0.3309569545563992 0.7502684637403526 0.5394923257002409  
0.0021983022240910 0.4997238666924472 0.4601119781054839  
0.5028183475090215 0.7505062359144348 0.4606674886799970  
0.4998112209452220 0.4991201210977599 0.3878940956806832  
0.0041200787364487 0.7486219193833746 0.3967495583547644  
0.3313379366230189 0.5011890681704801 0.4612428206459641  
0.1702960260478859 0.7505485381300534 0.4623927616126118  
0.8358893381295289 0.7483658723753976 0.4624012343063278  
0.1770002662099400 0.5002304031591184 0.3827989996709580  
0.8170131399281350 0.5074307514196938 0.3735959362428463  
0.6829121311879262 0.7507902232012993 0.3800853654785486  
0.3206563990532461 0.7507491447027013 0.3847888767445477  
0.5020332738413571 0.7509055233848718 0.6099142452628346  
0.0021630511710529 0.5002579122650168 0.6108596254038925  
0.0022132685917195 0.0010827281158764 0.6105788372139868  
0.6859725928013524 0.2490330228844907 0.3851388689608798  
0.3170629067239338 0.2508849862192870 0.3853676675629137  
0.5021051595404702 0.2498467967929917 0.6097100936039686  
0.5019453616052657 0.0006391602060651 0.5393561610810116  
0.0023506996278326 0.2500916470277534 0.5410591198130517  
0.6820867481989689 0.0006715513554026 0.6167600370844625  
0.3221018076992470 0.0001854915814906 0.6172600911550893  
0.1816180245543586 0.2508784001941698 0.6178206573553296  
0.8228486262701171 0.2501445164726985 0.6175447340657149  
0.1717350581265425 0.0006325434755371 0.5402503692071398  
0.8329267495370769 0.0006521256659636 0.5396599467081923  
0.6737599021615935 0.2502465432576023 0.5390721451722423  
0.6752207873926054 0.5020534597673409 0.4618586953359798  
0.0026491616930571 0.0024050034201220 0.4613997916766119  
0.8297303984493931 0.0005621233718973 0.3818751426921619  
0.3308206418229107 0.2505748822742065 0.5395484806133923  
0.1782379060267036 0.0008058700914949 0.3831293171393227  
0.1720687381128331 0.2505922244294465 0.4622314935041109  
0.3310920992921879 0.9999453621969147 0.4614045979420418  
0.8328422350847359 0.2528140514342121 0.4617887019514877  
0.0008273249214327 0.2539910966372612 0.3929701349431345  
0.5026176203324161 0.0025730341620577 0.3875314067316675  
0.5021253061998614 0.2493277775808168 0.4615504931157155  
0.6751647333842962 -0.0008494763960038 0.4609845460764583  
0.8428415826658270 0.7502573417390649 0.5391470249299781  
0.6585174476055359 0.7508711039225806 0.6195881647313751  
0.3459860368209819 0.7512081394323420 0.6209825581627870  
0.3425331258141075 0.5002343396573651 0.5383028781178341  
0.6618502202168907 0.5006021738857106 0.5388162471969696

0.1612094248100405 0.7504934038897282 0.5391237384222769  
0.6625181280882622 0.7508927515637956 0.4591248700908021  
0.1613812504326735 0.5002358510418853 0.4634423843898078  
0.3430982892940544 0.7505489315132793 0.4620091520465718  
0.1581973749179745 0.5000434060412278 0.6221424154175078  
0.3425612329226816 0.4988354736953743 0.3794610945831443  
0.6574241670143512 0.4943138295095654 0.3855391945544437  
0.8518759072555727 0.7489684337998969 0.3852679235600190  
0.8433546442774857 0.4999363012563105 0.4624370899603082  
0.8456634138827946 0.5000605421607257 0.6211910352856326  
0.6618648018076434 0.2503098613738926 0.4619599041336175  
0.8472052284163840 0.2559356482218527 0.3801903730514151  
0.6615586698912036 0.0019247195632486 0.3800248192505825  
0.3441992387383641 0.0021605272563037 0.3797543371540690  
0.3426858651060568 0.2502950402151501 0.4619612783914776  
0.1616654194355646 0.0009190873133051 0.4633170958236912  
0.8435354586874629 0.0012975491785273 0.4629721862993559  
0.1611040481607175 0.2506175953303472 0.5390850897661196  
0.8433043893161424 0.2510588538602778 0.5388649221277416  
0.6619212847155010 0.9998458358418799 0.5381336706313620  
0.6580059358596736 0.2498417565767762 0.6206901505910336  
0.3464069652456301 0.2496765478709977 0.6208647133842446  
0.1576215775606941 0.0009122363067309 0.6219983475748526  
0.8467390911502276 0.0008964743505365 0.6219687907598116  
0.1561285151312221 0.7509235183777746 0.3808532942900277  
0.1547676927266523 0.2501897624062303 0.3801115659336003  
0.3424644621974434 0.0004581325991216 0.5384624470861405  
0.7854961892072889 0.5668508109311301 0.3071260599926767  
0.7171372417936339 0.6879463590806307 0.3063268949904460  
0.6972042511333288 0.7320848628217105 0.2703309095773409

**N=NH site 4**

1.00000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 1

**Direct**

0.5016057415116713 0.4980754193882539 0.5395765619943974  
0.0015290725735535 0.7468707630237984 0.5404632522682125  
0.6826578147688059 0.4948849251407290 0.6179676456801031  
0.3194761866910176 0.4998498913128385 0.6171060719977282  
0.1790157245660682 0.7499473349575373 0.6172382054623374  
0.8240022825917110 0.7445475172337691 0.6178629029481724  
0.1705950472174497 0.4996963792998796 0.5389579272066033  
0.8320763353378631 0.4936392554247314 0.5392447960017928  
0.6731483049962343 0.7437566009241862 0.5404696905229334  
0.3299763985838685 0.7503542524038828 0.5399702943687442  
0.0012172089010993 0.4954414765712635 0.4599556183495911  
0.5017841102338744 0.7489305053264125 0.4633902531090551  
0.4970135792732004 0.5003440202370754 0.3780925516212292  
0.0007811457974936 0.7456765857665217 0.3924745800841403

0.3319618135575476 0.5013180051128816 0.4611193338998500  
0.1716873774821652 0.7515370839175879 0.4615136708278337  
0.8312783076212029 0.7412042549887012 0.4616921469079895  
0.1717527213819724 0.5029676261909179 0.3837763926579702  
0.8238891467897813 0.4879790298201787 0.3847716557998588  
0.6835169166661809 0.7392761991000520 0.3845712107577031  
0.3139287439963295 0.7572377843192140 0.3849322538394998  
0.5014621928906330 0.7470884043813609 0.6115927607652053  
0.0015958634030862 0.4975145302090780 0.6082972063943627  
0.0014648349015414 -0.0031538165776117 0.6085671542681503  
0.6740859126728173 0.2326096767740294 0.3768046428404768  
0.3255880488588402 0.2570384540604376 0.3777164756489717  
0.5014358052658106 0.2476483283980101 0.6140617986888935  
0.5013751955022522 -0.0045831020740646 0.5398143772132021  
0.0014964323682913 0.2467914108391403 0.5406779128320005  
0.6831972000026635 -0.0050169312400897 0.6174707029685161  
0.3206582275618046 -0.0002829468026261 0.6175427425319808  
0.1765778400332442 0.2493550550290720 0.6184298532633696  
0.8262933567608609 0.2453293529361479 0.6189606687465090  
0.1712829337854568 0.0002170470102266 0.5387599926536785  
0.8318361922176356 -0.0056134614790373 0.5393271855546676  
0.6720934760714270 0.2435961765142718 0.5405565127828420  
0.6683924175017364 0.4905911185917939 0.4609490715804610  
0.0025374217682117 -0.0022249854069146 0.4598319193249256  
0.8322453152311526 -0.0076155509512778 0.3848474213149875  
0.3309436140682047 0.2504725561132339 0.5401106893349225  
0.1792259055661108 0.0045815302366868 0.3834688611075863  
0.1729227309642209 0.2506228772956641 0.4605738627709161  
0.3335887253190288 0.0028782357776132 0.4604804353862276  
0.8296125922681041 0.2435690837303993 0.4603853950818061  
0.0015080636842301 0.2476545721097212 0.3901116265237459  
0.5072441983942654 0.0058415111667884 0.3819159186792822  
0.5022083300136503 0.2422150723212887 0.4643076603506150  
0.6732266839297928 -0.0076839503726780 0.4619111875208371  
0.8424018828817184 0.7442640664495173 0.5383865125027470  
0.6586611094636007 0.7447876606603463 0.6217390349849851  
0.3441790630978565 0.7494278895569414 0.6212632564661469  
0.3423449619098862 0.4998493466611793 0.5387866540940894  
0.6611538152171159 0.4933663049370771 0.5387021532299761  
0.1605240208264038 0.7499371263521062 0.5380336718972125  
0.6606724599603976 0.7418088604110176 0.4625595061456202  
0.1609195466850027 0.5005820194054921 0.4625092669311260  
0.3429059077674332 0.7524371784750774 0.4617301475126644  
0.1555305592373705 0.5007172517732313 0.6208171449159152  
0.3355636252443170 0.5148785043246362 0.3821341414800100  
0.6604061384933236 0.4922097376696442 0.3800907021345816  
0.8473719709259485 0.7374787514273388 0.3794559314329577  
0.8411647090833876 0.4926243221964635 0.4623276731330453  
0.8478523482427087 0.4955685509761549 0.6210123875950903  
0.6610875660651110 0.2418649018797363 0.4611288351434575  
0.8463124922632015 0.2422403973112005 0.3789003569915437  
0.6679018470546361 0.9808333414705157 0.3839059925029237

0.3435278719479794 0.9998113591791886 0.3802167105405626  
0.3429448303975678 0.2516964261451279 0.4616273762605409  
0.1621492732942970 0.0008782614686702 0.4618929886845406  
0.8431374970625365 -0.0068831322036168 0.4628339579770780  
0.1610387806860603 0.2497094412455859 0.5371702038504289  
0.8422219902220194 0.2440159032948224 0.5373965657339638  
0.6607694236635177 -0.0057581734324589 0.5395427957094557  
0.6600675579651311 0.2445968199377170 0.6218275304929647  
0.3425860506958515 0.2502575419283335 0.6211235006608891  
0.1556215249431749 -0.0012361393558480 0.6206908969959157  
0.8473178076924456 -0.0059984300425541 0.6211072316726498  
0.1528651685486022 0.7553603916214551 0.3785613257237397  
0.1576502827516769 0.2510422852688495 0.3786024588553961  
0.3420618378152301 0.0003062568441005 0.5384373637472366  
0.4633621773100603 0.3009359163397803 0.3306277239482867  
0.5455396024063137 0.1834583084559365 0.3342381045817495  
0.4407489793145066 0.3204009525151199 0.2930141570689900

**N=NH site 5**

1.0000000000000000  
12.0322999999999993 0.0000000000000000 0.0000000000000000  
-0.0000000007000000 8.0876000000000001 0.0000000000000000  
-0.0000000022000000 -0.0000000022000000 26.0656999999999996

Mn N H  
48 34 1

**Direct**

0.5015988498741368 0.5001348505161065 0.5390616687821771  
0.0014977290774666 0.7509008426805669 0.5411132775189055  
0.6798714179693958 0.5035247139629211 0.6181122461563719  
0.3227682493231082 0.4986487079059763 0.6180858223356105  
0.1790974760229760 0.7483773413872072 0.6177046553068436  
0.8242502575495649 0.7532643523881873 0.6174139683742886  
0.1708350401732700 0.4977725650865570 0.5396489981519914  
0.8317142571862831 0.5043681463287466 0.5393042224367081  
0.6721209338273406 0.7546378865593667 0.5395494359874264  
0.3303750974870331 0.7471682483075449 0.5396854308852822  
0.0010830749373373 0.5023445969654114 0.4600722947423428  
0.5012996319526980 0.7505002043544854 0.4654213279446947  
0.4961699197278217 0.5013698016088211 0.3772982453548101  
0.0024297146143540 0.7516034333093632 0.3922839518695621  
0.3308912421902380 0.4952422225191060 0.4611334092425206  
0.1739199814982050 0.7466947059902251 0.4608128584438515  
0.8297275870542367 0.7554414426724698 0.4610173701281642  
0.1705823594267779 0.4949580962771326 0.3832423202421280  
0.8254983678312946 0.5103444252480169 0.3831694966458511  
0.6808728067899869 0.7640263985202297 0.3761773920816986  
0.3272621293268350 0.7369039631194082 0.3790869043330383  
0.5016419031181372 0.7507902065511293 0.6102421688992984  
0.0015399771476685 0.4997613230717224 0.6108054095346515  
0.0014883728786421 0.0018704878528981 0.6108682249574787  
0.6909400247830468 0.2621876771654016 0.3845671053067660  
0.3137845724405464 0.2415886050985593 0.3853708587419076  
0.5015112266636036 0.2506770429107230 0.6090322418953190

0.5014760787831979 0.0013217868284546 0.5389976702599016  
0.0014716875380711 0.2508630226169059 0.5408331431337059  
0.6803522895214890 0.0031629350720758 0.6178306629377176  
0.3231209126673552 -0.0020764781641807 0.6182306792604790  
0.1819591799156112 0.2479088093740740 0.6166751732620397  
0.8211182538454593 0.2536983054441563 0.6164318672636628  
0.1712222391249370 -0.0026666431762806 0.5395254234472930  
0.8319272331949394 0.0041230357493129 0.5393599523613236  
0.6726046899265782 0.2545185845062223 0.5392543848232714  
0.6688751366505437 0.5084240350054313 0.4597831570304023  
0.0022195188073477 -0.0002159633828364 0.4602679914467205  
0.8337475391354251 0.0080795975679395 0.3833969973804770  
0.3299000344684859 0.2472421593268747 0.5397059557133002  
0.1780205632165149 -0.0074836720521351 0.3830047000289350  
0.1719382648585922 0.2452850338783327 0.4621285553137020  
0.3333405893066679 0.9943976113026731 0.4603540660610610  
0.8312431396914499 0.2567077892779597 0.4619425790335913  
0.0019866144330022 0.2512262234510236 0.3939267705288853  
0.5059914873007393 0.0099166542285850 0.3786074536875332  
0.5017689685204337 0.2501819251611831 0.4629449979488019  
0.6719951150094993 0.0058636581890445 0.4601778189765522  
0.8419864417362553 0.7541395005080012 0.5377123883229188  
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0.6598120258726089 0.7566752751218350 0.4607965853667995  
0.1607554378272672 0.4967724090816578 0.4630563267470871  
0.3427692257569520 0.7453274637198585 0.4599958352412779  
0.1573183767475030 0.4970158325363903 0.6214760640774164  
0.3341610999955985 0.4811431406811932 0.3828656165711304  
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0.8481590959983765 0.7563038907255802 0.3791920991685619  
0.8412937015643791 0.5059773709967401 0.4623618140218725  
0.8457242229758108 0.5024601468968115 0.6212313325905900  
0.6604906138978677 0.2572462804868715 0.4610772634268858  
0.8509810785546645 0.2611881632857682 0.3790745966901900  
0.6689504808864315 0.0206181304461036 0.3809164790939524  
0.3426527433619569 -0.0022559857256786 0.3799606442789882  
0.3429175430742718 0.2448480771566755 0.4617535474683326  
0.1618546659474211 -0.0037954614138071 0.4625822370760894  
0.8424054326592179 0.0054739936357451 0.4627356755678085  
0.1603140133882210 0.2477326969214686 0.5387443780852431  
0.8424302780742925 0.2541934393017653 0.5384941784129114  
0.6610694600572956 0.0042352131289042 0.5377553313374505  
0.6572062332372345 0.2534194697715014 0.6204577399978735  
0.3458510508067403 0.2480967751856354 0.6206621313812305  
0.1573305178770759 -0.0008366408464641 0.6214269497358789  
0.8456951103430567 0.0047997985899973 0.6213471875426473  
0.1568103874025830 0.7459088367214086 0.3797890241242033  
0.1531423900204044 0.2416229100840876 0.3793095893052816

0.3418524030031975 -0.0029159648558077 0.5378792936031827  
0.5371618525900236 0.8095085127008314 0.3322405780959465  
0.4546338273620765 0.6925180313830620 0.3354603641319278  
0.5540125751573085 0.8384104022746619 0.2944368947305158