

## **Prediction of improved magnetization and stability in Fe<sub>16</sub>N<sub>2</sub> through alloying**

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### **Supplementary Material**

**Table S1:** Equilibrium lattice parameters, in-plane  $a$  and out-of-plane  $c$ , as well as  $c/a$  and volume  $V$  for  $M_{16}N_2$  compounds, calculated using GGA. M represents the 3d transition metals Ti, V, Cr, Mn, Fe, Co, and Ni.

End-Member Lattice Parameters				
Compound	$a$ (Å)	$c$ (Å)	$c/a$	$V$ (Å <sup>3</sup> )
Fe <sub>16</sub> N <sub>2</sub>	5.67	6.23	1.09	200.48
Ti <sub>16</sub> N <sub>2</sub>	6.47	6.84	1.05	287.32
V <sub>16</sub> N <sub>2</sub>	5.94	6.46	1.08	228.06
Cr <sub>16</sub> N <sub>2</sub>	5.68	6.31	1.11	204.22
Mn <sub>16</sub> N <sub>2</sub>	5.14	7.23	1.40	191.12
Co <sub>16</sub> N <sub>2</sub>	5.70	5.70	1.00 (cubic)	185.43
Ni <sub>16</sub> N <sub>2</sub>	5.11	7.18	1.40	187.99

**Table S2:** Formation energies of  $\text{Fe}_{16-x}\text{M}_x\text{N}_2$  alloys calculated using GGA. M represents Ti, V, Cr, Mn, Co, and Ni. Alloy concentrations listed are given by  $(x/16) \times 100\%$ . Formation energies of end-member compounds, i.e. at M concentrations of 0% and 100%, are also listed. Values are normalized by dividing by the total number of atoms in the computational supercell, including both transition metal and nitrogen atoms.

Formation Energies (meV/atom)								
Element	0.00%	3.125%	6.25%	9.375%	12.5%	15.625%	18.75%	100.00%
Ti	-214	-243	-277	-300	-337	-345	-367	-779
V	-214	-235	-255	-272	-296	-302	-319	-726
Cr	-214	-214	-214	-215	-216	-217	-219	-448
Mn	-214	-215	-217	-219	-220	-223	-224	-541
Co	-214	-216	-219	-221	-223	-226	-229	-347
Ni	-214	-213	-213	-212	-212	-217	-221	-332

**Table S3:** Volume magnetization of  $\text{Fe}_{16-x}\text{M}_x\text{N}_2$  calculated using the hybrid HSE06 functional. M represents Ti, V, Cr, Mn, Co, and Ni. Alloy concentrations listed are given by  $(x/16) \times 100\%$ .

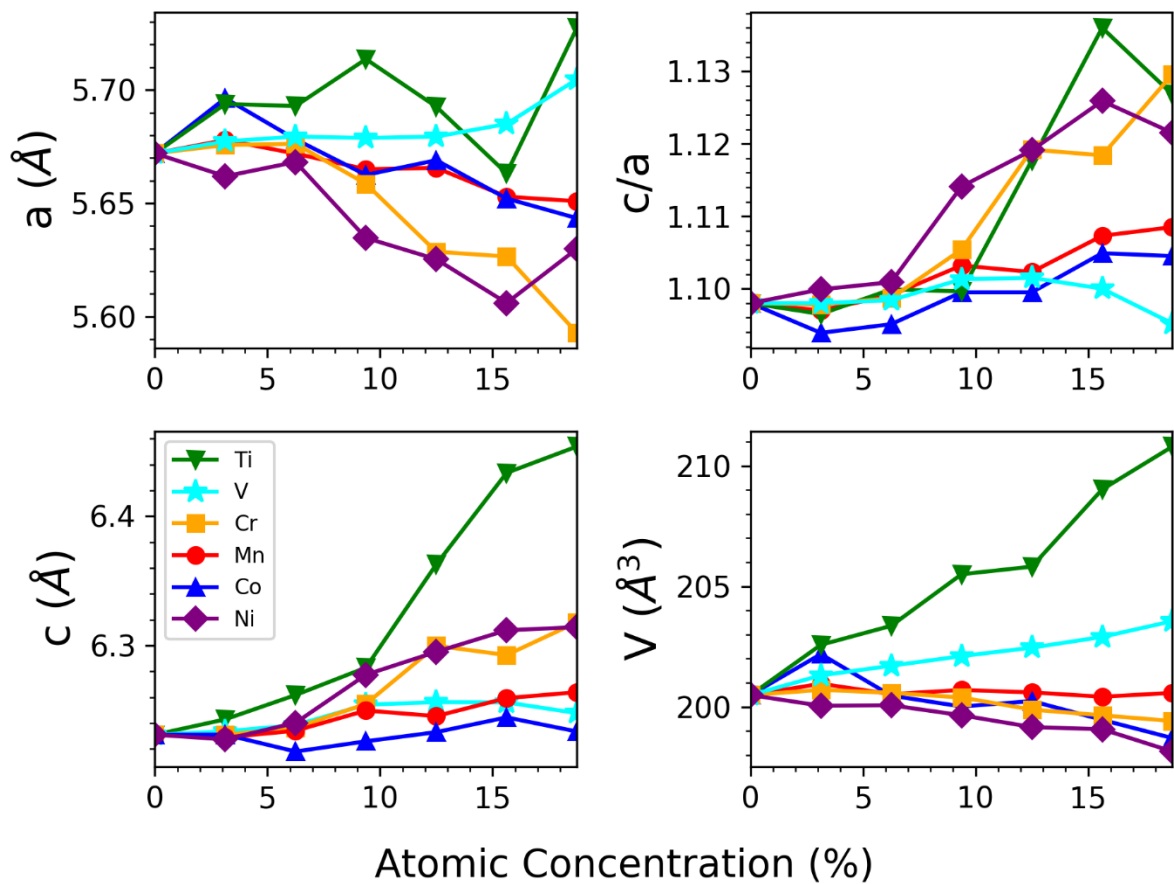
Volume Magnetization (MA/m)				
Element	0.00%	6.25%	12.5%	18.75%
Ti	2.103	1.824	1.600	1.364
V	2.103	1.816	1.558	1.321
Cr	2.103	1.780	1.508	1.442
Mn	2.103	2.104	2.104	2.103
Co	2.103	2.082	2.015	2.007
Ni	2.103	1.970	1.956	1.849

**Table S4:** Average  $-I_p\text{COHP}$  values for all bonds within each  $\text{Fe}_{14}\text{M}_2\text{N}_2$  alloy, calculated using GGA. M represents Ti, V, Cr, Mn, Co, and Ni. As only occupied states contribute to bonding and antibonding, all values are computed by integrating the COHP curves up to the Fermi energy. Units are arbitrary; however, comparison of magnitudes yields relative bond strengths and energies.

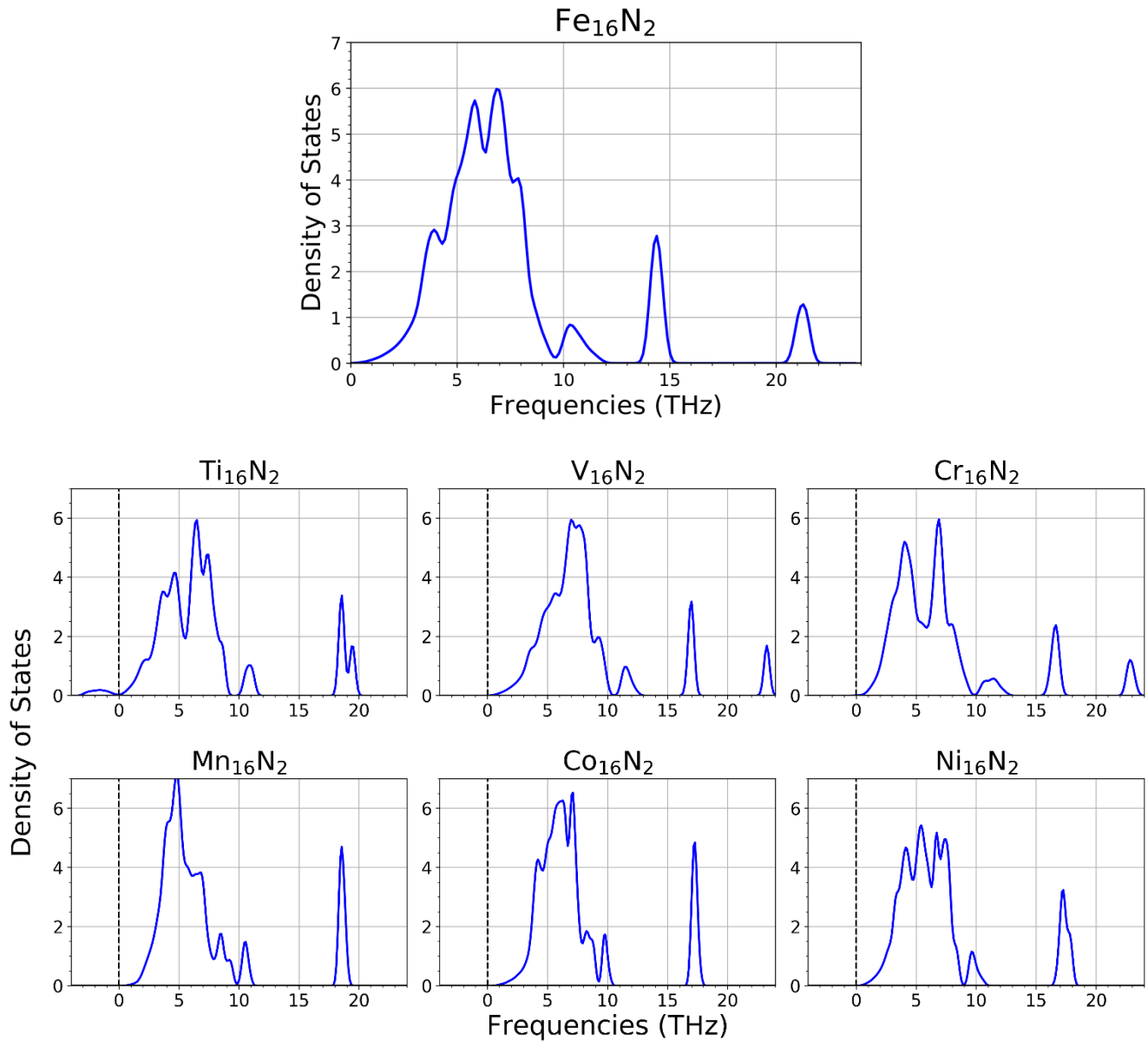
$-I_p\text{COHP}$ (eV)						
Pure	Ti	V	Cr	Mn	Co	Ni
0.994	1.075	1.051	1.041	1.029	1.034	1.008

**Table S5:** Average charge transfer of each element in  $\text{Fe}_{14}\text{M}_2\text{N}_2$ , calculated using the hybrid HSE06 functional. M represents Ti, V, Cr, Mn, Co, and Ni. Values are in units of electronic elementary charge ( $e$ ). Negative values indicate charge is received and positive values indicate charge is given away.

Charge Transfer ( $e$ )							
Element	Pure	Ti	V	Cr	Mn	Co	Ni
Fe	0.156	0.022	0.068	0.072	0.134	0.151	0.192
M	-	1.175	0.854	0.581	0.351	-0.015	-0.108
N	-1.243	-1.332	-1.331	-1.086	-1.288	-1.039	-1.238

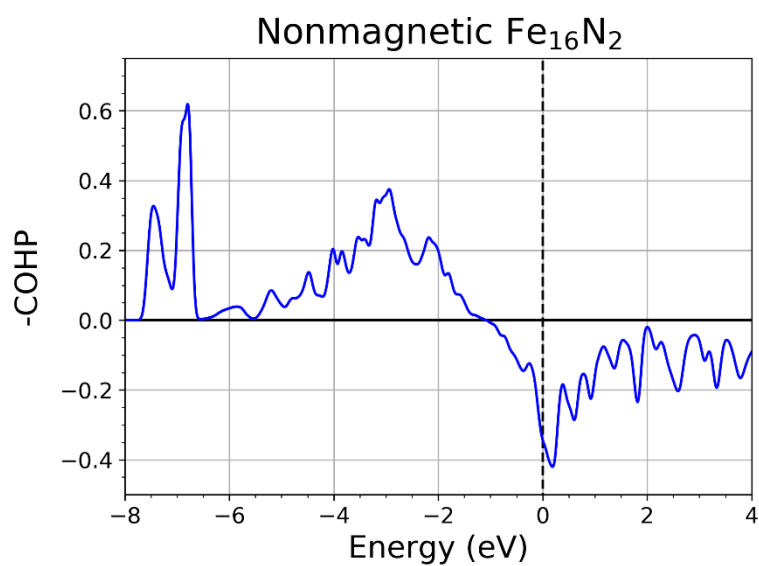


**Figure S1:** Structural parameters for  $\text{Fe}_{16-x}\text{M}_x\text{N}_2$  calculated using GGA. M represents Ti, V, Cr, Mn, Co, and Ni. Alloy concentrations listed are given by  $(x/16) \times 100\%$ .  $a$  and  $c$  represent unique in-plane and out-of-plane lattice constants, while  $V$  represents volume. Each point represents a calculated value, whereas the lines are interpolations.

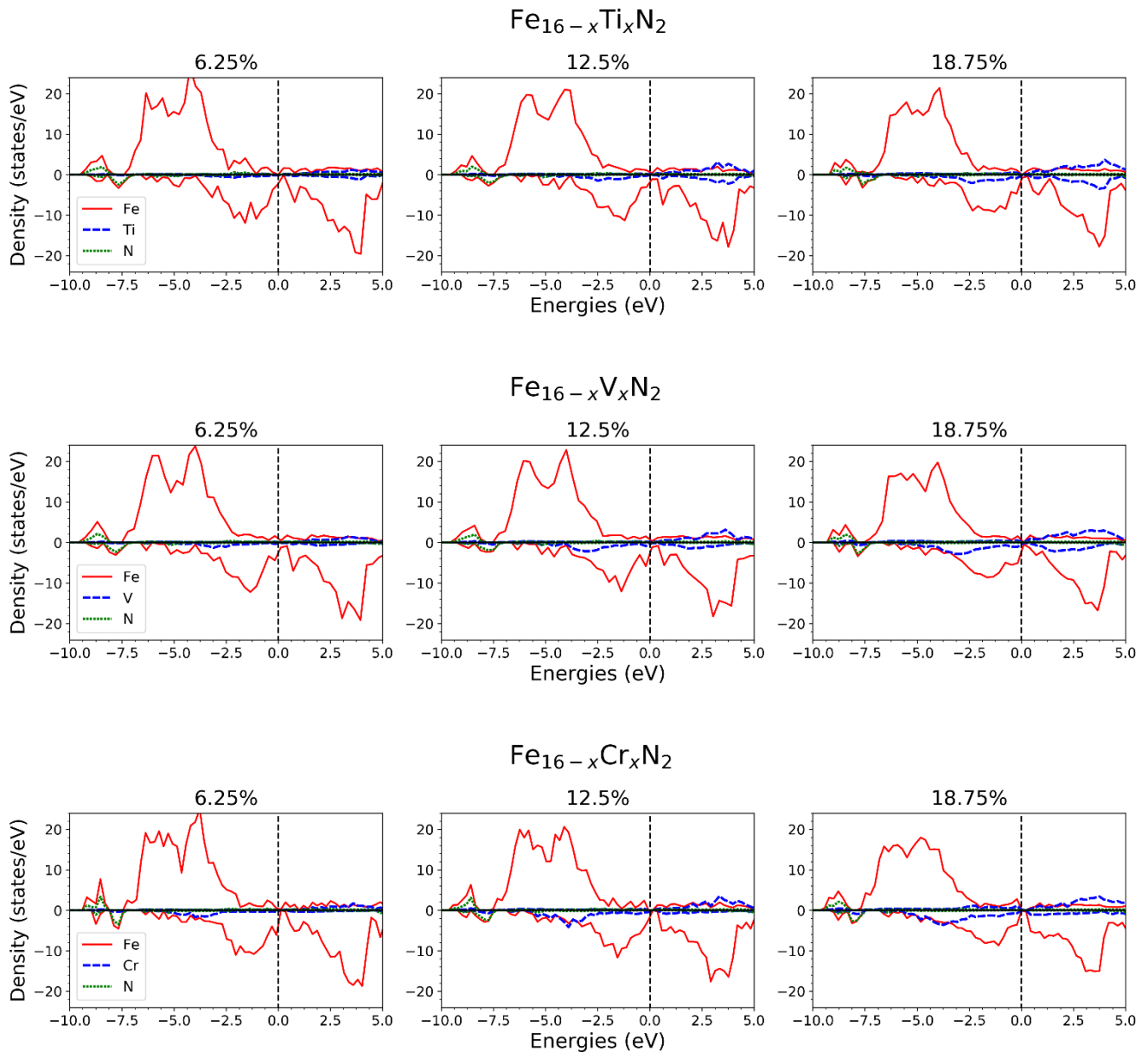


**Figure S2:** Phonon density of states for all end-member  $M_{16}N_2$  compounds calculated using GGA. M represents Ti, V, Cr, Mn, Co, and Ni. Values are normalized per formula unit. The dotted line represents zero frequency, which separates real (stable) and imaginary (unstable) frequencies.

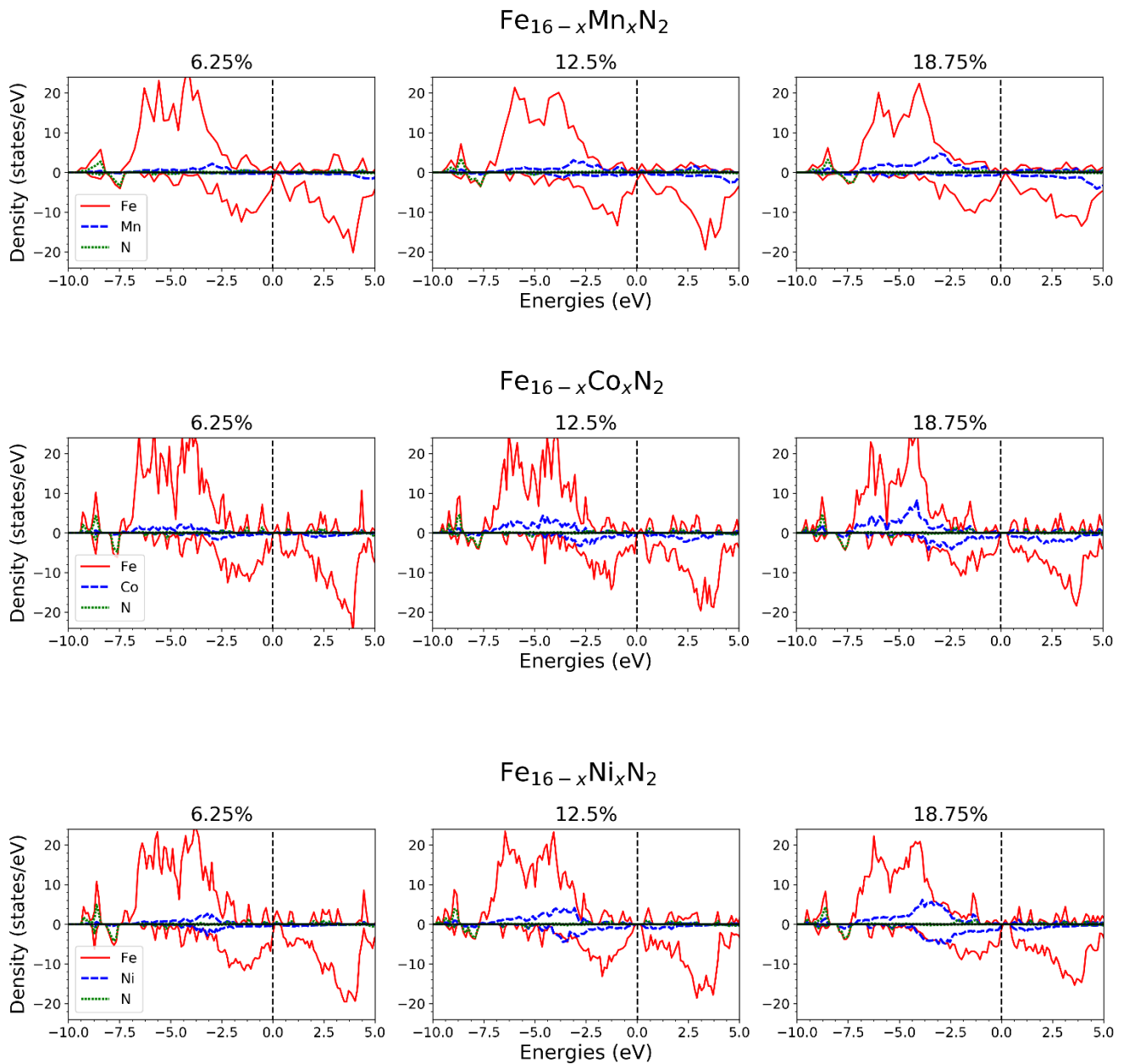




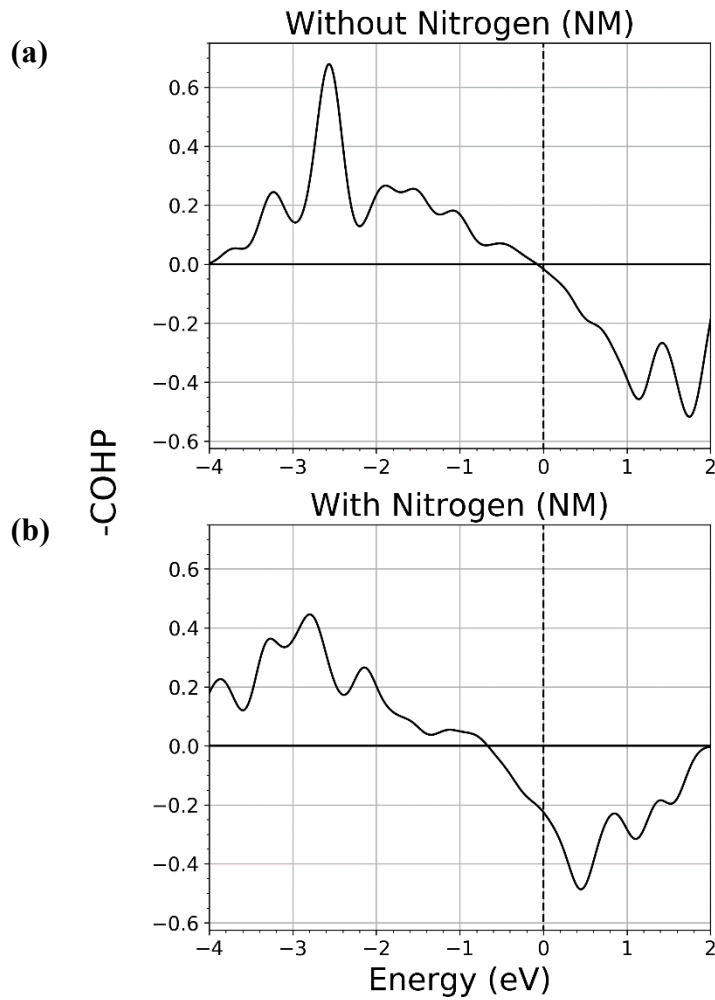
**Figure S3:** COHP curves of Fe<sub>16</sub>N<sub>2</sub> in the nonmagnetic configuration, calculated using the hybrid HSE06 functional. Positive -COHP values represent bonding, whereas negative values represent antibonding. The Fermi energy is set to 0 eV.



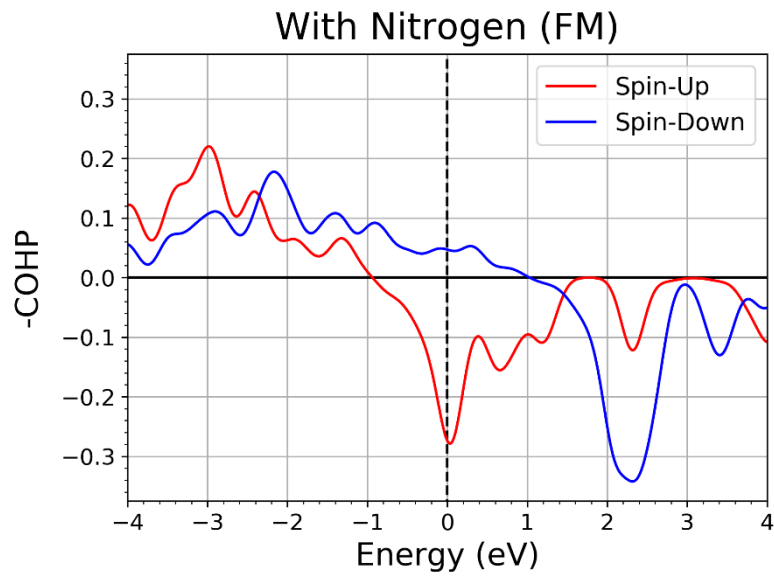
**Figure S4 (a):** Electronic density of states of  $\text{Fe}_{16-x}\text{M}_x\text{N}_2$  where M represents Ti, V, and Cr, i.e. the metals which couple antiferromagnetically with Fe. Alloy concentration is given by  $(x/16) \times 100\%$ . Positive spin densities are plotted above the x-axis, while negative spin densities are plotted below. The Fermi energy is set to 0 eV.



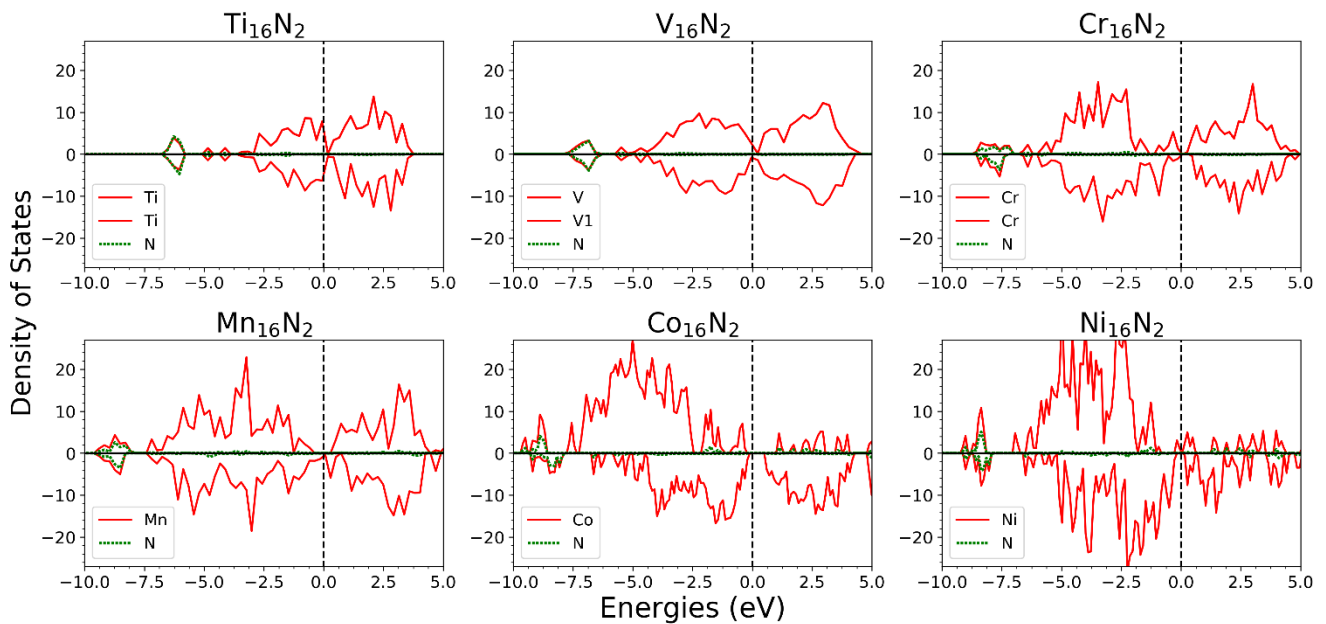
**Figure S4 (b):** Electronic density of states of  $\text{Fe}_{16-x}\text{Mn}_x\text{N}_2$  where M represents Mn, Ni, and Co, i.e. the metals which couple ferromagnetically with Fe. Alloy concentration is given by  $(x/16) \times 100\%$ . Positive spin densities are plotted above the x-axis, while negative spin densities are plotted below. The Fermi energy is set to 0 eV.



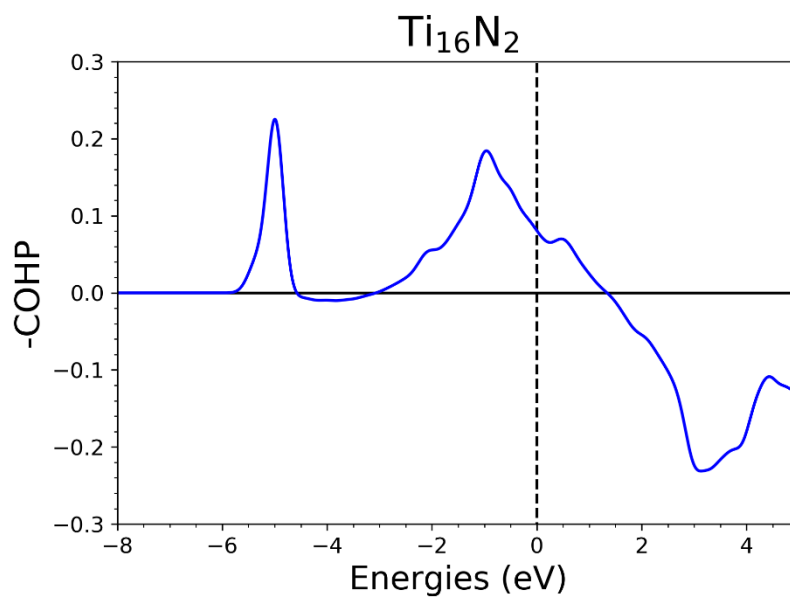
**Figure S5:** COHP curves, calculated using GGA, for isolated Mn atoms placed at the  $4d$  sites within  $\text{Fe}_{16}\text{N}_2$  (a) without and (b) with interstitial nitrogen atoms included. A nonmagnetic configuration is assumed in each case. Positive -COHP values represent bonding, whereas negative values represent antibonding. The Fermi energy is set to 0 eV.



**Figure S6:** Spin-polarized COHP curves, calculated using GGA, for isolated Mn atoms placed at the  $4d$  sites within  $\text{Fe}_{16}\text{N}_2$  with interstitial nitrogen atoms included. A ferromagnetic configuration is assumed. Positive -COHP values represent bonding, whereas negative values represent antibonding. The Fermi energy is set to 0 eV.



**Figure S7:** Electronic density of states of the end-member  $M_{16}N_2$  compounds calculated using the hybrid HSE06 functional. M represents the 3d transition metals Ti, V, Cr, Mn, Co, and Ni. Positive spin densities are plotted above the x-axis, while negative spin densities are plotted below. The Fermi energy is set to 0 eV.



**Figure S8:** COHP curves of Ti<sub>16</sub>N<sub>2</sub> calculated using GGA. Positive -COHP values represent bonding, whereas negative values represent antibonding. The Fermi energy is set to 0 eV.

## Special Quasirandom Structures (SQS) for $\text{Fe}_{16-x}\text{M}_x\text{N}_2$ (M = Ti, V, Cr, Mn, Co, Ni)

All structures are given in the standard POSCAR format used in VASP<sup>1</sup>

### Ti-alloys

**x/16 = 0.03125:**

```
Ti4 Fe124 N16
1.0
-5.693203 -0.000992 6.244368
5.693456 11.390658 -0.001588
-11.391874 0.004215 -12.493744
Fe N Ti
124 16 4
direct
0.499605 0.750534 0.624586 Fe
-0.001438 0.750314 0.375889 Fe
0.750760 0.249179 0.749682 Fe
0.248791 0.247079 0.496055 Fe
0.500507 0.750977 0.126421 Fe
0.000753 0.751222 0.875034 Fe
0.749441 0.248416 0.251455 Fe
0.248617 0.248981 0.000234 Fe
0.374891 -0.000318 0.562467 Fe
0.874269 0.000181 0.313012 Fe
0.628867 0.501168 0.687848 Fe
0.125006 0.500842 0.437468 Fe
0.374568 -0.000570 0.062066 Fe
0.874282 -0.000360 0.812496 Fe
0.621366 0.501943 0.188861 Fe
0.124869 0.499490 0.937562 Fe
0.249961 0.750348 0.750276 Fe
0.749732 0.750537 0.501518 Fe
0.499141 0.249478 0.874360 Fe
-0.004293 0.247950 0.624679 Fe
0.249745 0.750737 0.250096 Fe
0.750130 0.749504 -0.001243 Fe
0.500379 0.250262 0.374905 Fe
0.002727 0.248308 0.124411 Fe
0.124700 -0.000252 0.687538 Fe
0.624510 0.000775 0.438321 Fe
```

<sup>1</sup> [https://cms.mpi.univie.ac.at/vasp/vasp/POSCAR\\_file.html](https://cms.mpi.univie.ac.at/vasp/vasp/POSCAR_file.html)



0.873165 0.500148 0.562775 Fe  
0.126672 0.000235 0.186802 Fe  
0.624662 -0.000203 0.936912 Fe  
0.374068 0.499187 0.312944 Fe  
0.877785 0.501069 0.060182 Fe  
0.727758 0.750283 0.760979 Fe  
0.225988 0.750317 0.511865 Fe  
0.977068 0.249781 0.886405 Fe  
0.482351 0.245771 0.636033 Fe  
0.229144 0.750765 0.011097 Fe  
0.978644 0.249882 0.385771 Fe  
0.473783 0.247988 0.134895 Fe  
0.522672 0.750482 0.863995 Fe  
0.021293 0.750574 0.614455 Fe  
0.769618 0.247801 0.986517 Fe  
0.272694 0.247708 0.740493 Fe  
0.519251 0.751004 0.366137 Fe  
0.026965 0.750247 0.111911 Fe  
0.772771 0.249978 0.488604 Fe  
0.273533 0.250496 0.239091 Fe  
0.854319 0.000128 0.574341 Fe  
0.353991 0.001453 0.323568 Fe  
0.101883 0.501925 0.699121 Fe  
0.602129 0.498849 0.449565 Fe  
0.852720 0.000140 0.072737 Fe  
0.352562 -0.000390 0.823187 Fe  
0.108807 0.502110 0.200019 Fe  
0.603605 0.499246 0.947950 Fe  
0.646756 -0.000495 0.676105 Fe  
0.146813 -0.000545 0.425946 Fe  
0.898473 0.498968 0.801363 Fe  
0.396011 0.502356 0.549587 Fe  
0.648479 -0.000082 0.176619 Fe  
0.146680 -0.000654 0.926295 Fe  
0.900942 0.504299 0.305062 Fe  
0.398813 0.500406 0.051868 Fe  
0.816740 0.878356 0.908636 Fe  
0.316896 0.878268 0.658885 Fe  
0.066390 0.378093 0.034572 Fe  
0.569781 0.376567 0.782324 Fe  
0.814278 0.880411 0.413476 Fe  
0.320350 0.879383 0.158758 Fe  
0.065006 0.378473 0.532373 Fe  
0.570742 0.378720 0.282982 Fe  
0.938649 0.121098 0.969339 Fe  
0.438813 0.120420 0.719793 Fe  
0.191658 0.621282 0.094113 Fe  
0.694398 0.622239 0.843645 Fe

0.939914 0.121649 0.469680 Fe  
0.439994 0.122059 0.219464 Fe  
0.186755 0.622939 0.594637 Fe  
0.683463 0.620479 0.348994 Fe  
0.810535 0.377958 0.904861 Fe  
0.060871 0.878668 0.029962 Fe  
0.560221 0.878061 0.780223 Fe  
0.811015 0.378367 0.405615 Fe  
0.311425 0.378444 0.155314 Fe  
0.060993 0.878810 0.530650 Fe  
0.554445 0.880600 0.283566 Fe  
0.434092 0.623152 0.715177 Fe  
0.930987 0.621998 0.467366 Fe  
0.681953 0.120658 0.840056 Fe  
0.183956 0.121172 0.591492 Fe  
0.424755 0.621095 0.218826 Fe  
0.933450 0.621380 0.965113 Fe  
0.682978 0.121644 0.341427 Fe  
0.180991 0.120585 0.091042 Fe  
0.942411 0.127644 0.721659 Fe  
0.442674 0.128192 0.470982 Fe  
0.189910 0.630472 0.848157 Fe  
0.692216 0.628576 0.596992 Fe  
0.943381 0.128385 0.220830 Fe  
0.440201 0.126882 0.970037 Fe  
0.193915 0.629580 0.346919 Fe  
0.694812 0.627308 0.094062 Fe  
0.064153 0.369620 0.781055 Fe  
0.561921 0.370547 0.533030 Fe  
0.315512 0.872088 0.906887 Fe  
0.813833 0.871849 0.657669 Fe  
0.064078 0.372332 0.282685 Fe  
0.562911 0.371607 0.030948 Fe  
0.313411 0.872192 0.407381 Fe  
0.817305 0.872565 0.155117 Fe  
0.935716 0.629246 0.718491 Fe  
0.436636 0.629610 0.467466 Fe  
0.184563 0.127420 0.843262 Fe  
0.686794 0.127627 0.592537 Fe  
0.939872 0.627649 0.217193 Fe  
0.435495 0.630720 0.971102 Fe  
0.185156 0.127960 0.341899 Fe  
0.684938 0.126735 0.092550 Fe  
0.557545 0.872302 0.528933 Fe  
0.061550 0.873104 0.278259 Fe  
0.808452 0.371287 0.653334 Fe  
0.307095 0.371258 0.403166 Fe  
0.558365 0.872030 0.028726 Fe

0.057558 0.871872 0.778797 Fe  
0.304285 0.369719 0.905851 Fe  
0.499329 -0.001010 0.749604 N  
0.002396 0.001465 0.500862 N  
0.749982 0.499314 0.874081 N  
0.247903 0.504200 0.624061 N  
0.500863 0.001373 0.249644 N  
-0.000957 -0.000607 -0.000874 N  
0.749431 0.498988 0.375877 N  
0.249784 0.498656 0.123866 N  
0.626124 0.249612 0.561842 N  
0.124904 0.250053 0.311732 N  
0.874751 0.750756 0.687847 N  
0.372527 0.751418 0.439079 N  
0.618373 0.245661 0.059135 N  
0.124338 0.249312 0.813038 N  
0.881406 0.749866 0.184482 N  
0.376364 0.750982 0.937760 N  
0.377269 0.504450 0.818275 Ti  
0.728988 0.750677 0.261223 Ti  
0.310371 0.373159 0.648841 Ti

**x/16 = 0.0625:**

Ti4 Fe60 N8

1.0

5.692918 -5.687555 6.261677

-5.693427 -5.679065 6.270125

0.008747 -5.702476 -6.283104

Fe N Ti

60 8 4

direct

0.436972 0.439376 0.622274 Fe

0.188042 0.186862 0.124913 Fe

0.933377 0.937277 0.627523 Fe

0.689196 0.686716 0.120055 Fe

0.561434 0.065019 0.378747 Fe

0.064276 0.563299 0.374496 Fe

0.814676 0.312958 0.871919 Fe

0.310645 0.310846 0.877910 Fe

0.059657 0.067140 0.368345 Fe

0.811895 0.813572 0.877691 Fe

0.564705 0.557865 0.373087 Fe

0.438570 0.940081 0.629676 Fe

0.187616 0.686306 0.123306 Fe

0.938809 0.438004 0.624571 Fe

0.687057 0.186174 0.127394 Fe

0.177167 0.674822 0.646413 Fe

0.929003 0.428712 0.143473 Fe  
0.674477 0.175128 0.651411 Fe  
0.421232 0.928749 0.143460 Fe  
0.074203 0.574796 0.852408 Fe  
0.572134 0.075309 0.856573 Fe  
0.319697 0.821100 0.346625 Fe  
0.427456 0.423045 0.146197 Fe  
0.173344 0.184768 0.648414 Fe  
0.923641 0.927357 0.147366 Fe  
0.679598 0.674739 0.649954 Fe  
0.323426 0.323892 0.353789 Fe  
0.072675 0.075039 0.857544 Fe  
0.826089 0.823125 0.355359 Fe  
0.572300 0.574068 0.851713 Fe  
0.934603 0.688455 0.623811 Fe  
0.684573 0.439571 0.111351 Fe  
0.432387 0.191034 0.625915 Fe  
0.176296 0.939843 0.124583 Fe  
0.815329 0.570954 0.373599 Fe  
0.560607 0.321916 0.880032 Fe  
0.308619 0.067690 0.379688 Fe  
0.058630 0.818959 0.877068 Fe  
0.940597 0.185496 0.112335 Fe  
0.688375 0.933003 0.627088 Fe  
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0.319303 0.554019 0.877843 Fe  
0.073659 0.314368 0.373341 Fe  
0.813705 0.063580 0.880717 Fe  
0.182632 0.438379 0.122166 Fe  
0.932439 0.188710 0.626495 Fe  
0.679511 0.938438 0.125943 Fe  
0.435785 0.689086 0.614540 Fe  
0.060483 0.317777 0.879805 Fe  
0.810690 0.065119 0.379999 Fe  
0.563382 0.819027 0.876497 Fe  
0.311814 0.565038 0.375946 Fe  
0.939630 0.682525 0.121172 Fe  
0.687360 0.432591 0.625348 Fe  
0.438453 0.180589 0.124861 Fe  
0.565731 0.309371 0.380484 Fe  
0.316643 0.064400 0.876439 Fe  
0.066487 0.810513 0.374295 Fe  
0.818189 0.559482 0.878940 Fe  
0.252825 0.248853 0.501027 N  
0.996414 -0.000769 0.998784 N  
0.756694 0.748256 0.506732 N  
0.500958 0.495100 0.997100 N

0.499653 0.999550 0.000809 N  
0.251974 0.743295 0.495119 N  
0.002109 0.501745 0.998012 N  
0.747769 0.246191 0.507674 N  
0.316115 0.806896 0.882505 Ti  
0.823535 0.323441 0.353764 Ti  
0.567091 0.810932 0.377901 Ti  
0.184704 0.939168 0.610919 Ti

**x/16 = 0.09375:**

Ti12 Fe116 N16

1.0

0.001900 -11.442123 0.009376  
-11.427205 0.001897 -0.001682  
-0.001917 0.010518 -12.573448

Fe N Ti

116 16 12

direct

0.753514 0.501145 0.373755 Fe  
0.249699 0.498982 0.372711 Fe  
0.249655 -0.000724 0.372164 Fe  
0.749093 0.499964 0.874720 Fe  
0.750797 0.999974 0.875370 Fe  
0.251387 0.497591 0.878407 Fe  
0.246816 0.002631 0.874869 Fe  
0.497384 0.243974 0.374985 Fe  
0.497348 0.754155 0.368709 Fe  
0.000332 0.247294 0.375002 Fe  
0.998643 0.751185 0.374191 Fe  
0.501228 0.250897 0.874863 Fe  
0.000446 0.249643 0.874635 Fe  
0.997889 0.752220 0.878449 Fe  
0.752070 0.500021 0.628256 Fe  
0.752322 0.000296 0.626029 Fe  
0.251972 0.501258 0.625665 Fe  
0.249043 0.999417 0.627872 Fe  
0.752225 0.000601 0.123407 Fe  
0.248418 0.499640 0.124239 Fe  
0.245470 0.001579 0.123946 Fe  
0.498191 0.248057 0.632892 Fe  
0.497543 0.753024 0.627748 Fe  
0.998031 0.248965 0.629891 Fe  
-0.000903 0.752316 0.623344 Fe  
0.500197 0.249687 0.119264 Fe  
0.502269 0.747660 0.124703 Fe  
0.000744 0.250701 0.122763 Fe  
-0.000203 0.748463 0.123975 Fe

0.752740 0.755661 0.395022 Fe  
0.755480 0.242770 0.397448 Fe  
0.249119 0.749316 0.392749 Fe  
0.750812 0.751020 0.897386 Fe  
0.749739 0.250379 0.898024 Fe  
0.247965 0.749099 0.900153 Fe  
0.249998 0.249907 0.898640 Fe  
0.754543 0.753563 0.605017 Fe  
0.754059 0.246614 0.606860 Fe  
0.251694 0.248191 0.608654 Fe  
0.751004 0.750023 0.101996 Fe  
0.752892 0.249664 0.101538 Fe  
0.243755 0.744717 0.102334 Fe  
0.248429 0.250531 0.097930 Fe  
0.499128 0.503872 0.145189 Fe  
0.504747 0.001891 0.143399 Fe  
0.000191 0.499478 0.147669 Fe  
0.000595 0.998562 0.145326 Fe  
0.496514 0.500899 0.649679 Fe  
0.499482 0.998198 0.651836 Fe  
0.993060 0.500483 0.647767 Fe  
0.001164 -0.001543 0.648116 Fe  
0.492357 0.501424 0.352031 Fe  
0.997665 0.501092 0.352540 Fe  
0.000920 0.001175 0.352310 Fe  
0.501715 0.498747 0.852472 Fe  
0.503859 0.001662 0.851714 Fe  
0.996243 0.495317 0.855048 Fe  
-0.000355 0.000674 0.853688 Fe  
0.622427 0.877977 0.503888 Fe  
0.121014 0.881246 0.491915 Fe  
0.624414 0.879256 0.001573 Fe  
0.621186 0.378593 0.999708 Fe  
0.119380 0.877768 -0.000025 Fe  
0.120941 0.378590 0.999214 Fe  
0.378387 0.879641 0.495151 Fe  
0.376577 0.376960 0.507605 Fe  
0.881575 0.879412 0.502475 Fe  
0.875115 0.376757 0.499495 Fe  
0.379260 0.379216 -0.000398 Fe  
0.878273 0.878768 -0.000036 Fe  
0.879693 0.376914 0.997307 Fe  
0.118775 0.622814 0.496846 Fe  
0.122601 0.120248 0.508159 Fe  
0.622630 0.121694 0.505538 Fe  
0.119815 0.619225 0.998047 Fe  
0.120279 0.121249 0.998736 Fe  
0.621742 0.621216 -0.001044 Fe

0.624233 0.123033 0.999802 Fe  
0.875896 0.624564 0.500270 Fe  
0.882788 0.122153 0.504689 Fe  
0.376052 0.620979 0.492706 Fe  
0.380156 0.118416 0.516517 Fe  
0.879657 0.621810 0.995907 Fe  
0.879431 0.121778 0.998901 Fe  
0.377122 0.620437 0.001426 Fe  
0.379462 0.123509 -0.002262 Fe  
0.369571 0.629386 0.247523 Fe  
0.370643 0.129057 0.234134 Fe  
0.872286 0.630072 0.251553 Fe  
0.875664 0.128409 0.244071 Fe  
0.371493 0.626312 0.751909 Fe  
0.370548 0.128241 0.754487 Fe  
0.871341 0.628380 0.753164 Fe  
0.871709 0.127658 0.752325 Fe  
0.126722 0.627289 0.251428 Fe  
0.126889 0.127633 0.246355 Fe  
0.628153 0.629420 0.254899 Fe  
0.630996 0.128313 0.243232 Fe  
0.127935 0.128908 0.750612 Fe  
0.631435 0.628006 0.744695 Fe  
0.629798 0.128298 0.750576 Fe  
0.874042 0.370260 0.252229 Fe  
0.873822 0.870724 0.244867 Fe  
0.371658 0.372324 0.243972 Fe  
0.367463 0.870143 0.239681 Fe  
0.870575 0.370614 0.751192 Fe  
0.873208 0.871813 0.752035 Fe  
0.370463 0.371771 0.752970 Fe  
0.370626 0.874467 0.755979 Fe  
0.629972 0.870305 0.242555 Fe  
0.127146 0.371531 0.251178 Fe  
0.127012 0.871024 0.250005 Fe  
0.629325 0.371423 0.749397 Fe  
0.632388 0.872109 0.748021 Fe  
0.127480 0.371903 0.749879 Fe  
0.126250 0.873705 0.754075 Fe  
0.494588 0.498765 0.500355 N  
0.502086 -0.000190 0.505402 N  
0.991860 0.504513 0.500357 N  
0.001179 0.001271 0.500193 N  
0.501147 0.500456 -0.000974 N  
0.505667 0.004137 0.997528 N  
-0.000043 0.499031 0.001045 N  
-0.000464 0.000190 -0.000338 N  
0.248084 0.251518 0.242937 N

0.246880 0.749318 0.247591 N  
0.755967 0.247046 0.250127 N  
0.750838 0.750335 0.249247 N  
0.248646 0.250893 0.753246 N  
0.252534 0.753545 0.754675 N  
0.749407 0.249828 0.752199 N  
0.751775 0.750366 0.750772 N  
0.754614 0.000041 0.374206 Ti  
0.506301 0.746464 0.871083 Ti  
0.754918 0.503857 0.120362 Ti  
0.260126 0.237667 0.394236 Ti  
0.252182 0.754734 0.601499 Ti  
0.493977 0.002392 0.351826 Ti  
0.620490 0.373043 0.501901 Ti  
0.117952 0.380662 0.505721 Ti  
0.373953 0.882267 0.004935 Ti  
0.619744 0.626605 0.499592 Ti  
0.125107 0.626364 0.755179 Ti  
0.623860 0.367162 0.254635 Ti

**x/16 = 0.125:**

Ti4 Fe28 N4

1.0

0.002586 -5.680452 6.372471

0.001110 5.671740 6.364406

-5.695605 0.005092 -6.370166

Fe N Ti

28 4 4

direct

0.377636 0.873259 0.001129 Fe

0.871624 0.870952 0.491968 Fe

0.375196 0.371816 0.497849 Fe

0.129085 0.627576 0.007818 Fe

0.623754 0.126527 -0.000870 Fe

0.625132 0.631066 0.497142 Fe

0.126683 0.121236 0.497202 Fe

0.599222 0.110923 0.500769 Fe

0.108280 0.591108 0.497868 Fe

0.887061 0.388765 0.484682 Fe

0.362957 0.351279 0.004183 Fe

0.853333 0.855043 0.004628 Fe

0.151485 0.150157 0.011073 Fe

0.643068 0.641659 -0.008333 Fe

0.498597 0.261634 0.758652 Fe

0.251398 0.493504 0.756329 Fe

0.765113 0.005404 0.757320 Fe

0.740143 0.500905 0.241506 Fe

0.245660 0.002936 0.242681 Fe



0.505894 0.748735 0.239507 Fe  
-0.006915 0.234688 0.243548 Fe  
0.260374 0.506568 0.257331 Fe  
0.742617 0.003705 0.248845 Fe  
0.005803 0.752043 0.258392 Fe  
0.504863 0.260962 0.273315 Fe  
0.496632 0.750274 0.747795 Fe  
0.249074 0.990290 0.750653 Fe  
0.752474 0.500052 0.737131 Fe  
-0.002043 0.006513 0.006074 N  
0.495918 0.500747 -0.001941 N  
0.739989 0.250313 0.489576 N  
0.244831 0.741770 0.500324 N  
0.872740 0.379585 0.008733 Ti  
0.398221 0.896311 0.503878 Ti  
0.002280 0.754446 0.755479 Ti

**x/16 = 0.15625:**

Ti20 Fe108 N16

1.0

0.015619 -11.499279 6.347785  
0.018090 -11.477037 -6.306925  
11.493706 5.727227 -0.012496

Fe N Ti

108 16 20

direct

0.128552 0.870665 0.504182 Fe  
0.752900 0.496417 0.999212 Fe  
0.873774 0.623621 0.502430 Fe  
0.499629 0.254901 0.997312 Fe  
0.624589 0.380349 0.498980 Fe  
0.246076 0.001751 0.998732 Fe  
0.377172 0.124389 0.501571 Fe  
0.062414 0.817127 0.752155 Fe  
0.687404 0.437306 0.249635 Fe  
0.811471 0.563562 0.750712 Fe  
0.428280 0.190222 0.249861 Fe  
0.312580 0.058664 0.747906 Fe  
0.877530 0.127453 0.502303 Fe  
0.499052 0.749274 0.997969 Fe  
0.624409 0.874457 0.501982 Fe  
0.254745 0.498171 0.999425 Fe  
0.375539 0.625926 0.496221 Fe  
0.998576 0.250704 0.001385 Fe  
0.121904 0.376097 0.499618 Fe  
0.687856 0.932664 0.246983 Fe  
0.812099 0.061887 0.752243 Fe

0.445251 0.684648 0.253202 Fe  
0.560428 0.814708 0.748897 Fe  
0.190671 0.431941 0.254732 Fe  
0.315126 0.562140 0.753066 Fe  
0.938295 0.188994 0.250057 Fe  
0.059440 0.314339 0.749249 Fe  
0.912549 0.711630 0.753452 Fe  
0.043445 0.828164 0.247394 Fe  
0.666256 0.464712 0.755038 Fe  
0.791842 0.580736 0.244753 Fe  
0.418124 0.208420 0.747081 Fe  
0.538807 0.340089 0.248628 Fe  
0.286610 0.088805 0.248600 Fe  
0.709455 0.914936 0.747889 Fe  
0.461758 0.666603 0.751359 Fe  
0.208177 0.417296 0.748844 Fe  
0.343404 0.536124 0.256415 Fe  
0.958242 0.170128 0.751345 Fe  
0.083352 0.289698 0.250568 Fe  
0.102483 0.389569 0.999827 Fe  
0.225167 0.519449 0.492489 Fe  
0.852282 0.147418 0.000303 Fe  
0.596768 0.898603 0.996159 Fe  
0.727541 0.019188 0.501910 Fe  
0.359385 0.645680 0.996390 Fe  
0.478602 0.773246 0.499594 Fe  
0.026634 0.730745 0.500885 Fe  
0.648292 0.351879 0.999382 Fe  
0.767425 0.481989 0.502000 Fe  
0.389414 0.099189 0.994589 Fe  
0.516211 0.225990 0.502296 Fe  
0.146916 0.854089 0.994608 Fe  
0.277917 0.977227 0.503873 Fe  
0.715768 0.716865 0.622138 Fe  
0.838451 0.838177 0.116347 Fe  
0.599567 0.579069 0.117382 Fe  
0.222169 0.215280 0.624528 Fe  
0.341827 0.338667 0.122011 Fe  
0.956881 0.975747 0.621619 Fe  
0.085571 0.096236 0.118870 Fe  
0.593786 0.597804 0.622364 Fe  
0.717212 0.718754 0.118557 Fe  
0.336520 0.349419 0.620157 Fe  
0.469235 0.472251 0.120139 Fe  
0.092369 0.100684 0.625578 Fe  
0.215846 0.220158 0.121649 Fe  
0.850352 0.843138 0.627089 Fe  
0.978927 0.963858 0.118728 Fe

0.531119 0.532273 0.879055 Fe  
0.662757 0.648557 0.380035 Fe  
0.409331 0.398548 0.377117 Fe  
0.021891 0.038778 0.879001 Fe  
0.158438 0.157619 0.380614 Fe  
0.773352 0.782610 0.874325 Fe  
0.906042 0.908092 0.382565 Fe  
0.910629 0.911096 0.876983 Fe  
0.652222 0.662895 0.876596 Fe  
0.404242 0.414013 0.878847 Fe  
0.536888 0.535285 0.380184 Fe  
0.153660 0.162629 0.879137 Fe  
0.280798 0.283176 0.379282 Fe  
0.911744 0.391999 0.869452 Fe  
0.025307 0.529038 0.371966 Fe  
0.653397 0.151449 0.869405 Fe  
0.774904 0.283145 0.371425 Fe  
0.403749 0.901374 0.870048 Fe  
0.528298 0.028082 0.371436 Fe  
0.159686 0.651677 0.872731 Fe  
0.278951 0.781307 0.373720 Fe  
0.784991 0.280185 0.873802 Fe  
0.899037 0.415142 0.370354 Fe  
0.523305 0.037711 0.868134 Fe  
0.282929 0.779817 0.870213 Fe  
0.410687 0.906889 0.374390 Fe  
0.043594 0.520268 0.872216 Fe  
0.160119 0.656754 0.373203 Fe  
0.715837 0.221360 0.126823 Fe  
0.836011 0.351367 0.631223 Fe  
0.462930 0.970579 0.125753 Fe  
0.596476 0.087078 0.627502 Fe  
0.346336 0.838877 0.626605 Fe  
0.973866 0.460414 0.130480 Fe  
0.228201 0.712883 0.626682 Fe  
0.846543 0.345774 0.129024 Fe  
0.964079 0.481609 0.633936 Fe  
0.344591 0.845958 0.122771 Fe  
0.473091 0.970618 0.629101 Fe  
0.742073 0.755501 0.996820 N  
0.879479 0.877615 0.507492 N  
0.501745 0.498033 0.998693 N  
0.623940 0.628861 0.501750 N  
0.250010 0.247994 0.004969 N  
0.370879 0.371687 0.496588 N  
0.001051 0.001110 0.999851 N  
0.134001 0.125262 0.505391 N  
0.937986 0.435890 0.251208 N

0.061728 0.565295 0.757740 N  
0.684289 0.192874 0.247338 N  
0.810363 0.317481 0.754781 N  
0.429977 0.944656 0.249352 N  
0.562775 0.061372 0.749874 N  
0.196009 0.685620 0.257679 N  
0.315656 0.807368 0.748078 N  
0.994748 0.752649 0.993900 Ti  
0.938146 0.688268 0.250552 Ti  
0.558718 0.311109 0.758066 Ti  
0.194505 0.942576 0.249234 Ti  
0.751827 0.997541 0.990500 Ti  
0.163963 0.958438 0.748934 Ti  
0.835326 0.037283 0.243490 Ti  
0.574526 0.786904 0.241288 Ti  
0.979321 0.278456 0.504522 Ti  
0.888786 0.596806 0.989501 Ti  
0.462201 0.471835 0.616593 Ti  
0.281204 0.278724 0.877125 Ti  
0.044523 0.026499 0.387943 Ti  
0.783426 0.786623 0.387658 Ti  
0.649970 0.161114 0.373133 Ti  
0.234858 0.706815 0.129018 Ti  
0.092520 0.594424 0.629170 Ti  
0.117259 0.576527 0.131785 Ti  
0.579089 0.105857 0.123986 Ti  
0.725789 0.217929 0.627017 Ti

**x/16 = 0.1875:**

Ti12 Fe52 N8

1.0

11.528780 -0.054598 6.334952

11.513443 5.729233 -0.022396

-0.020686 5.747509 6.325301

Fe N Ti

52 8 12

direct

0.369547 0.626862 0.879194 Fe

0.624639 0.877217 0.626168 Fe

0.878234 0.117767 0.375614 Fe

0.133006 0.368191 0.122547 Fe

0.252677 0.996326 -0.002140 Fe

0.755159 0.492846 0.497726 Fe

0.004722 0.752051 0.253605 Fe

0.125384 0.874009 0.629891 Fe

0.620911 0.374416 0.125524 Fe

0.873362 0.627477 0.867288 Fe

0.002493 0.250239 0.742809 Fe  
0.251432 0.496094 0.501324 Fe  
0.744872 0.008219 0.996374 Fe  
0.235395 0.521131 0.973624 Fe  
0.468599 0.775461 0.741690 Fe  
0.731854 0.023019 0.470565 Fe  
0.029173 0.725472 0.763619 Fe  
0.272952 0.975140 0.531702 Fe  
0.520586 0.227232 0.273940 Fe  
0.772722 0.479841 0.018147 Fe  
0.353356 0.642269 0.360090 Fe  
0.853164 0.143056 0.847525 Fe  
0.100960 0.399827 0.600489 Fe  
0.385311 0.110357 0.899887 Fe  
0.646066 0.346682 0.650151 Fe  
0.903192 0.599829 0.399331 Fe  
0.177198 0.943397 0.816621 Fe  
0.432464 0.187622 0.575760 Fe  
0.692103 0.934191 0.313592 Fe  
0.923068 0.196546 0.040597 Fe  
0.183023 0.436748 0.809672 Fe  
0.441058 0.677721 0.572067 Fe  
0.557669 0.317616 0.435163 Fe  
0.059053 0.818853 0.936750 Fe  
0.311834 0.065750 0.697193 Fe  
0.314006 0.565990 0.679126 Fe  
0.812436 0.065810 0.176785 Fe  
0.060105 0.319735 0.916978 Fe  
0.066886 0.804889 0.449647 Fe  
0.305606 0.064821 0.196148 Fe  
0.558069 0.313571 0.947947 Fe  
0.806273 0.566372 0.691925 Fe  
0.818704 0.054021 0.681623 Fe  
0.057325 0.312158 0.433445 Fe  
0.320291 0.550739 0.192609 Fe  
0.559812 0.812304 0.929766 Fe  
0.942425 0.688372 0.559878 Fe  
0.190425 0.932949 0.333056 Fe  
0.428684 0.203947 0.058088 Fe  
0.450224 0.676815 0.061448 Fe  
0.941057 0.184380 0.555977 Fe  
0.189216 0.444723 0.298788 Fe  
0.993775 0.005643 0.995803 N  
0.247557 0.253417 0.746046 N  
0.496410 0.499568 0.508751 N  
0.753161 0.751628 0.256279 N  
0.129420 0.119280 0.389134 N  
0.374497 0.376931 0.126580 N

0.623741 0.629803 0.877026 N  
0.881418 0.872812 0.616689 N  
0.490976 0.263034 0.746655 Ti  
0.360870 0.144302 0.379538 Ti  
0.482470 0.761127 0.247505 Ti  
0.005421 0.238158 0.212975 Ti  
0.594151 0.907448 0.108606 Ti  
0.146931 0.856725 0.147148 Ti  
0.941696 0.688624 0.066047 Ti  
0.684314 0.428526 0.321206 Ti  
0.823078 0.558984 0.186500 Ti  
0.578085 0.798818 0.453574 Ti  
0.684622 0.443034 0.810908 Ti  
0.698624 0.931068 0.795693 Ti

## V-alloys

**x/16 = 0.03125:**

V4 Fe124 N16  
1.0  
11.358659 -0.010067 12.472777  
0.001629 -5.689181 12.475891  
11.361072 -5.687200 0.002394  
Fe N V  
124 16 4  
direct  
0.811975 0.312544 0.188023 Fe  
0.812857 0.812499 0.687263 Fe  
0.062995 0.561993 0.937073 Fe  
0.312700 0.311892 0.187323 Fe  
0.061150 0.063707 0.438320 Fe  
0.312206 0.813077 0.687972 Fe  
0.562798 0.562910 0.936914 Fe  
0.187943 0.937095 0.062288 Fe  
0.186277 0.438379 0.563128 Fe  
0.437339 0.187843 0.812027 Fe  
0.687376 0.937271 0.062379 Fe  
0.437767 0.686335 0.312807 Fe  
0.688142 0.437695 0.562273 Fe  
0.937936 0.187725 0.812151 Fe  
0.937528 0.687399 0.312274 Fe  
0.688294 0.186778 0.312333 Fe  
0.686926 0.688614 0.812724 Fe  
0.937170 0.437225 0.062784 Fe  
0.187810 0.188422 0.311844 Fe

0.938034 0.936763 0.562095 Fe  
0.187659 0.686860 0.812554 Fe  
0.437118 0.437401 0.062695 Fe  
0.437292 0.937708 0.562762 Fe  
0.062582 0.812357 0.187355 Fe  
0.062937 0.312779 0.687653 Fe  
0.312284 0.062317 0.938292 Fe  
0.564047 0.811036 0.186303 Fe  
0.311349 0.565169 0.437533 Fe  
0.561271 0.312954 0.687935 Fe  
0.811903 0.062298 0.938340 Fe  
0.813205 0.562094 0.436984 Fe  
0.676333 0.426395 0.074232 Fe  
0.676731 0.926370 0.572477 Fe  
0.926443 0.676417 0.823193 Fe  
0.176266 0.426372 0.073849 Fe  
0.926146 0.176754 0.323828 Fe  
0.175470 0.926513 0.576625 Fe  
0.426141 0.676894 0.823751 Fe  
0.427345 0.174546 0.322429 Fe  
0.574405 0.323837 0.174155 Fe  
0.573166 0.824196 0.676438 Fe  
0.823460 0.573526 0.927006 Fe  
0.073940 0.323034 0.176195 Fe  
0.823940 0.072947 0.425467 Fe  
0.074115 0.822589 0.676154 Fe  
0.322427 0.573993 0.926684 Fe  
0.324388 0.074367 0.428254 Fe  
0.176130 0.176176 0.823523 Fe  
0.176204 0.676819 0.323609 Fe  
0.426927 0.426838 0.574491 Fe  
0.675293 0.175965 0.824619 Fe  
0.427343 0.926498 0.072058 Fe  
0.676560 0.675671 0.323438 Fe  
0.927909 0.427943 0.572248 Fe  
0.925887 0.926746 0.074146 Fe  
0.073344 0.073434 0.926207 Fe  
0.073997 0.574181 0.426107 Fe  
0.324690 0.321454 0.675575 Fe  
0.573733 0.073996 0.926265 Fe  
0.323279 0.823113 0.176016 Fe  
0.573929 0.573229 0.426583 Fe  
0.823162 0.822977 0.176792 Fe  
0.689219 0.311219 0.933001 Fe  
0.689197 0.810278 0.431898 Fe  
0.938520 0.561016 0.682801 Fe  
0.188687 0.310628 0.933237 Fe  
0.939433 0.060891 0.182217 Fe

0.189735 0.812532 0.431376 Fe  
0.439671 0.561758 0.682341 Fe  
0.438710 0.058872 0.183063 Fe  
0.933089 0.065376 0.689429 Fe  
0.933139 0.566396 0.188897 Fe  
0.182636 0.317626 0.439215 Fe  
0.431655 0.067893 0.689891 Fe  
0.182303 0.817430 0.939219 Fe  
0.432275 0.568120 0.189045 Fe  
0.682484 0.317228 0.439445 Fe  
0.682462 0.817490 0.939108 Fe  
0.317818 0.682464 0.560951 Fe  
0.317785 0.182310 0.060623 Fe  
0.569029 0.930553 0.309966 Fe  
0.817246 0.683366 0.560451 Fe  
0.565016 0.433556 0.812020 Fe  
0.817443 0.182425 0.061175 Fe  
0.067442 0.932881 0.310753 Fe  
0.067194 0.433122 0.811156 Fe  
0.559641 0.438411 0.319247 Fe  
0.561577 0.940310 0.815927 Fe  
0.811757 0.688886 0.066740 Fe  
0.060876 0.439158 0.317595 Fe  
0.809967 0.188100 0.566981 Fe  
0.059472 0.938753 0.819162 Fe  
0.310493 0.688231 0.067655 Fe  
0.312568 0.191251 0.567033 Fe  
0.189268 0.061298 0.682419 Fe  
0.189054 0.560765 0.182174 Fe  
0.689230 0.060912 0.681822 Fe  
0.439097 0.810797 0.932448 Fe  
0.688476 0.560577 0.183079 Fe  
0.941057 0.311763 0.430983 Fe  
0.938661 0.810777 0.933129 Fe  
0.433485 0.816218 0.438978 Fe  
0.431490 0.318165 0.939448 Fe  
0.681478 0.067072 0.191356 Fe  
0.932538 0.817273 0.439025 Fe  
0.684006 0.568854 0.687669 Fe  
0.931911 0.317647 0.939476 Fe  
0.182139 0.067369 0.189649 Fe  
0.182820 0.566692 0.689321 Fe  
0.817954 0.431877 0.311000 Fe  
0.818211 0.931908 0.810603 Fe  
0.066502 0.682890 0.061406 Fe  
0.316342 0.433820 0.310644 Fe  
0.067828 0.184705 0.560211 Fe  
0.317738 0.932786 0.810577 Fe



0.567198 0.682276 0.060821 Fe  
0.567506 0.182078 0.559714 Fe  
0.060623 0.188717 0.067615 Fe  
0.061407 0.689124 0.567319 Fe  
0.310236 0.438552 0.817707 Fe  
0.560469 0.188990 0.068023 Fe  
0.560878 0.689427 0.567896 Fe  
0.812260 0.440720 0.816207 Fe  
0.810523 0.939048 0.317803 Fe  
-0.000010 -0.000180 0.000289 N  
0.000585 0.501479 0.499117 N  
0.247825 0.251379 0.752389 N  
0.500695 0.000010 -0.001100 N  
0.249708 0.750134 0.249758 N  
0.500159 0.500196 0.500540 N  
0.749206 0.249457 0.750176 N  
0.751902 0.747103 0.248916 N  
0.499332 0.750639 0.750532 N  
0.499645 0.250207 0.249982 N  
0.750502 -0.000395 0.500214 N  
0.000449 0.749328 0.750160 N  
0.749018 0.500595 0.001299 N  
0.000537 0.249194 0.249038 N  
0.250573 -0.000327 0.500365 N  
0.249100 0.500421 0.000033 N  
0.565650 0.055443 0.437397 V  
0.823523 0.323440 0.676400 V  
0.436135 0.318243 0.432634 V  
0.310569 0.939078 0.316906 V

**$x/16 = 0.0625$ :**

V4 Fe60 N8

1.0

-0.003126 -5.689978 6.246210

0.001461 -5.683798 -6.240564

11.361838 0.001668 -0.004202

Fe N V

60 8 4

direct

0.874629 0.623679 -0.000429 Fe

0.875248 0.625007 0.499894 Fe

0.375032 0.125299 0.500014 Fe

0.624477 0.375206 0.249316 Fe

0.624357 0.376238 0.749758 Fe

0.126411 0.873612 0.250344 Fe

0.125195 0.874672 0.750493 Fe

0.624002 0.874292 -0.000265 Fe

0.625268 0.875531 0.499599 Fe  
0.124542 0.375673 0.000246 Fe  
0.124430 0.375095 0.500113 Fe  
0.374655 0.625527 0.250442 Fe  
0.375443 0.624507 0.750229 Fe  
0.874098 0.126378 0.250945 Fe  
0.876284 0.125469 0.747974 Fe  
0.853836 0.646806 0.751062 Fe  
0.853150 0.644655 0.250088 Fe  
0.351732 0.146690 0.751368 Fe  
0.353722 0.147008 0.248852 Fe  
0.647155 0.849185 0.747676 Fe  
0.646373 0.852678 0.251305 Fe  
0.147731 0.352871 0.750624 Fe  
0.147203 0.352280 0.250050 Fe  
0.854311 0.149364 -0.000113 Fe  
0.352343 0.647384 0.000147 Fe  
0.351926 0.648374 0.500401 Fe  
0.644148 0.351831 0.000549 Fe  
0.643892 0.355694 0.500098 Fe  
0.149922 0.853294 -0.001322 Fe  
0.148432 0.851691 0.500492 Fe  
0.622645 0.620158 0.620881 Fe  
0.620861 0.622966 0.122191 Fe  
0.123998 0.121790 0.622728 Fe  
0.122058 0.121319 0.122570 Fe  
0.378461 0.378079 0.621966 Fe  
0.377698 0.379499 0.121639 Fe  
0.879414 0.875893 0.622142 Fe  
0.120299 0.122338 0.878891 Fe  
0.124109 0.120448 0.376741 Fe  
0.622449 0.621302 0.879011 Fe  
0.621842 0.621251 0.378084 Fe  
0.876211 0.880224 0.877597 Fe  
0.879017 0.875947 0.377067 Fe  
0.380531 0.376594 0.879440 Fe  
0.378200 0.377957 0.378104 Fe  
0.619288 0.125197 0.371347 Fe  
0.121989 0.621414 0.872063 Fe  
0.121441 0.620611 0.371383 Fe  
0.379659 0.879271 0.872313 Fe  
0.378126 0.879634 0.371796 Fe  
0.878149 0.378854 0.871545 Fe  
0.875607 0.380443 0.372014 Fe  
0.120140 0.622941 0.128323 Fe  
0.121727 0.620784 0.629159 Fe  
0.623266 0.118621 0.127902 Fe  
0.619960 0.124250 0.626683 Fe

0.877943 0.378106 0.128447 Fe  
0.875461 0.381211 0.628543 Fe  
0.379548 0.878620 0.128593 Fe  
0.378970 0.878322 0.628599 Fe  
0.500364 0.501531 0.000502 N  
0.497319 0.501572 0.499333 N  
-0.000782 -0.001030 -0.000302 N  
0.001513 -0.001095 0.499462 N  
0.500580 -0.000374 0.250420 N  
0.500400 -0.000985 0.749561 N  
0.001305 0.499605 0.249209 N  
0.001493 0.500031 0.750461 N  
0.368727 0.125652 0.003183 V  
0.853202 0.146945 0.500288 V  
0.877109 0.876724 0.121999 V  
0.629754 0.121390 0.868172 V

**x/16 = 0.09375:**

V12 Fe116 N16

1.0

0.001075 -11.374712 6.251679

0.002032 -11.379346 -6.260166

11.357464 5.686964 0.001234

Fe N V

116 16 12

direct

-0.001583 0.750002 -0.000555 Fe

0.125712 0.873945 0.499861 Fe

0.749934 0.501412 0.000582 Fe

0.874888 0.623930 0.499681 Fe

0.499031 0.251265 -0.000014 Fe

0.626840 0.373471 0.501065 Fe

0.374692 0.125743 0.500022 Fe

0.937769 0.687316 0.250126 Fe

0.064378 0.811329 0.751425 Fe

0.686826 0.437454 0.248349 Fe

0.812055 0.563036 0.750184 Fe

0.437158 0.188034 0.249533 Fe

0.561032 0.312315 0.750712 Fe

0.189445 0.936828 0.250098 Fe

0.311992 0.062706 0.749583 Fe

0.748924 -0.000152 -0.000269 Fe

0.500935 0.749147 -0.000326 Fe

0.625128 0.874803 0.499716 Fe

0.249350 0.500580 0.001426 Fe

0.374089 0.626306 0.500030 Fe

0.001384 0.250219 0.000544 Fe

0.124883 0.373763 0.498879 Fe  
0.687604 0.938411 0.250345 Fe  
0.811843 0.062066 0.750835 Fe  
0.562115 0.812085 0.749514 Fe  
0.187744 0.437819 0.250135 Fe  
0.312801 0.562634 0.750158 Fe  
0.936663 0.189238 0.251068 Fe  
0.062121 0.311786 0.749110 Fe  
0.911935 0.709607 0.748464 Fe  
0.040602 0.835043 0.250716 Fe  
0.665429 0.460777 0.749477 Fe  
0.790111 0.584321 0.250124 Fe  
0.539516 0.334255 0.248386 Fe  
0.167586 0.958839 0.751374 Fe  
0.290559 0.085129 0.249087 Fe  
0.709087 0.914533 0.750169 Fe  
0.832176 0.042956 0.250774 Fe  
0.459706 0.666112 0.750575 Fe  
0.583853 0.790807 0.249856 Fe  
0.206445 0.414329 0.748952 Fe  
0.334470 0.542347 0.250020 Fe  
0.960230 0.166293 0.748212 Fe  
0.084294 0.290870 0.250082 Fe  
0.102818 0.397623 0.000774 Fe  
0.229515 0.519586 0.498536 Fe  
0.853001 0.148457 0.000942 Fe  
0.977928 0.270365 0.498943 Fe  
0.602710 0.896395 0.000456 Fe  
0.728658 0.022366 0.498879 Fe  
0.356084 0.646083 0.001894 Fe  
0.477303 0.771933 0.497843 Fe  
0.896519 0.603536 0.000225 Fe  
0.647339 0.352500 0.000276 Fe  
0.774749 0.477665 0.502055 Fe  
0.396395 0.103971 0.000405 Fe  
0.523921 0.224888 0.499389 Fe  
0.272159 0.976680 0.498557 Fe  
0.714419 0.717024 0.621031 Fe  
0.840833 0.841712 0.122626 Fe  
0.592164 0.590300 0.121341 Fe  
0.214322 0.216316 0.620617 Fe  
0.340595 0.342810 0.121880 Fe  
0.092946 0.092240 0.123286 Fe  
0.594379 0.594865 0.622694 Fe  
0.719798 0.719823 0.122764 Fe  
0.341782 0.346756 0.621831 Fe  
0.467853 0.472139 0.121902 Fe  
0.095446 0.092534 0.620769 Fe

0.219459 0.220638 0.121738 Fe  
0.843705 0.844559 0.622704 Fe  
0.532319 0.528136 0.878443 Fe  
0.653861 0.655146 0.376882 Fe  
0.278356 0.282257 0.878472 Fe  
0.406701 0.405132 0.377740 Fe  
0.028963 0.033033 0.878251 Fe  
0.156327 0.153652 0.377279 Fe  
0.779332 0.780923 0.879241 Fe  
0.905157 0.907879 0.378001 Fe  
0.909148 0.906853 0.877685 Fe  
0.034392 0.033328 0.378785 Fe  
0.659155 0.658611 0.879076 Fe  
0.781678 0.784228 0.377488 Fe  
0.403432 0.413912 0.878947 Fe  
0.159007 0.159445 0.878805 Fe  
0.283565 0.283809 0.377722 Fe  
0.904658 0.404602 0.873134 Fe  
0.029757 0.526055 0.370607 Fe  
0.655137 0.152807 0.873188 Fe  
0.775691 0.280865 0.370321 Fe  
0.403686 0.904022 0.871891 Fe  
0.529565 0.028869 0.371719 Fe  
0.279257 0.776676 0.369716 Fe  
0.906297 0.406970 0.371314 Fe  
0.532463 0.030264 0.872653 Fe  
0.655327 0.159456 0.371113 Fe  
0.283858 0.781445 0.872565 Fe  
0.407025 0.908238 0.370946 Fe  
0.031023 0.531415 0.872301 Fe  
0.160154 0.654393 0.372167 Fe  
0.718411 0.217125 0.128000 Fe  
0.843048 0.342955 0.628779 Fe  
0.467871 0.968406 0.128567 Fe  
0.595239 0.091563 0.628078 Fe  
0.215574 0.718874 0.127501 Fe  
0.342375 0.842618 0.627447 Fe  
0.967153 0.468428 0.128543 Fe  
0.095432 0.589909 0.627663 Fe  
0.094543 0.598057 0.128816 Fe  
0.223125 0.719527 0.629410 Fe  
0.846486 0.346404 0.128794 Fe  
0.973022 0.468657 0.627745 Fe  
0.596268 0.095227 0.127407 Fe  
0.722384 0.221022 0.630158 Fe  
0.350696 0.845775 0.129901 Fe  
0.470880 0.969506 0.626524 Fe  
0.750141 0.750414 0.001181 N

0.876298 0.874488 0.500051 N  
0.501273 0.497806 -0.001243 N  
0.625623 0.624203 0.499813 N  
0.250068 0.251367 0.000488 N  
0.377264 0.371773 0.498894 N  
-0.001622 0.000737 -0.000366 N  
0.125643 0.123765 0.498700 N  
0.936718 0.437201 0.249427 N  
0.059149 0.562949 0.749033 N  
0.685002 0.188245 0.247669 N  
0.813006 0.314008 0.751032 N  
0.438949 0.940215 0.251507 N  
0.562588 0.061306 0.749774 N  
0.185346 0.687349 0.249360 N  
0.313625 0.812852 0.749878 N  
0.251252 0.003526 -0.000755 V  
0.871613 0.129833 0.496800 V  
0.434503 0.691650 0.246654 V  
0.415869 0.210335 0.750331 V  
0.022565 0.723026 0.498360 V  
0.150746 0.856860 0.002537 V  
0.468054 0.465680 0.622298 V  
0.968310 0.966664 0.626466 V  
0.967004 0.970457 0.125384 V  
0.537134 0.528034 0.380511 V  
0.155086 0.649028 0.870686 V  
0.782443 0.282279 0.873306 V

**x/16 = 0.125:**

V4 Fe28 N4  
1.0  
-0.007172 -5.686847 6.271144  
-0.006138 5.677277 6.262329  
-5.678972 0.004273 -6.260651  
Fe N V  
28 4 4  
direct  
0.375383 0.874558 0.000036 Fe  
0.875620 0.875070 0.500275 Fe  
0.374319 0.376051 0.500266 Fe  
0.124793 0.625626 0.000891 Fe  
0.626540 0.123164 -0.001028 Fe  
0.625402 0.627047 0.501656 Fe  
0.122428 0.124118 0.497932 Fe  
0.607112 0.103237 0.503353 Fe  
0.101942 0.603627 0.497449 Fe  
0.397856 0.895879 0.499286 Fe

0.900240 0.398799 0.501048 Fe  
0.349026 0.355266 0.002111 Fe  
0.145680 0.146311 -0.001939 Fe  
0.647758 0.645930 0.003429 Fe  
0.001323 0.756034 0.753827 Fe  
0.256054 0.502493 0.756006 Fe  
0.755485 0.000562 0.755040 Fe  
0.740320 0.497044 0.240763 Fe  
0.248239 0.001620 0.244900 Fe  
0.499820 0.743734 0.243808 Fe  
0.001600 0.245331 0.244073 Fe  
0.249729 0.508479 0.259564 Fe  
0.748997 0.003159 0.255008 Fe  
0.006898 0.748757 0.259060 Fe  
0.491102 0.747469 0.744494 Fe  
0.992036 0.250390 0.741353 Fe  
0.252517 0.995792 0.742633 Fe  
0.745732 0.489164 0.742741 Fe  
0.001747 -0.000542 -0.000151 N  
0.496585 0.498701 -0.000084 N  
0.751058 0.250617 0.499317 N  
0.253437 0.753836 0.504750 N  
0.882624 0.379258 0.005606 V  
0.853352 0.849926 -0.002115 V  
0.490999 0.252992 0.750135 V  
0.506249 0.250501 0.254503 V

**x/16 = 0.15625:**

V20 Fe108 N16

1.0

-0.004497 5.694058 12.532981

-0.009877 -5.692799 12.532387

11.387863 0.005068 -6.272927

Fe N V

108 16 20

direct

0.813987 0.313484 0.001401 Fe

0.937437 0.436845 0.498772 Fe

0.187038 0.688132 0.500826 Fe

0.313959 0.813187 0.001858 Fe

0.561025 0.063373 0.998120 Fe

0.686428 0.188501 0.501151 Fe

0.124404 0.126437 0.250216 Fe

0.249184 0.251465 0.749421 Fe

0.374708 0.375040 0.250453 Fe

0.501459 0.499478 0.748847 Fe

0.627124 0.625302 0.251043 Fe

0.750040 0.747299 0.747455 Fe  
0.001794 0.999306 0.748396 Fe  
0.688659 0.184202 0.998703 Fe  
0.811857 0.309959 0.498477 Fe  
0.937639 0.435964 0.998506 Fe  
0.064031 0.562606 0.500437 Fe  
0.312678 0.813102 0.499899 Fe  
0.562513 0.063549 0.501844 Fe  
0.000753 0.000323 0.251340 Fe  
0.122531 0.123798 0.749783 Fe  
0.249665 0.252491 0.249377 Fe  
0.373605 0.374729 0.748411 Fe  
0.499695 0.499644 0.249867 Fe  
0.622176 0.625616 0.751435 Fe  
0.749604 0.752830 0.251422 Fe  
0.876914 0.873841 0.750243 Fe  
0.738853 0.239069 0.751665 Fe  
0.864603 0.364303 0.250011 Fe  
0.113372 0.614610 0.251754 Fe  
0.238083 0.740580 0.748825 Fe  
0.368061 0.862975 0.251142 Fe  
0.486475 0.988427 0.747035 Fe  
0.612411 0.115561 0.251602 Fe  
0.634626 0.135374 0.748073 Fe  
0.761130 0.261587 0.251208 Fe  
0.883441 0.384029 0.750004 Fe  
0.014236 0.508960 0.251621 Fe  
0.136217 0.637993 0.751013 Fe  
0.387754 0.883910 0.751912 Fe  
0.513821 0.010484 0.247019 Fe  
0.179164 0.173713 0.001695 Fe  
0.302943 0.302599 0.501263 Fe  
0.425338 0.428842 0.001676 Fe  
0.549268 0.550552 0.498218 Fe  
0.671575 0.679750 0.997951 Fe  
0.801899 0.804114 0.500791 Fe  
0.047549 0.051974 0.496867 Fe  
0.076593 0.073881 0.001563 Fe  
0.197659 0.199192 0.499848 Fe  
0.323188 0.324825 0.000012 Fe  
0.449053 0.448423 0.500183 Fe  
0.823574 0.821852 -0.000394 Fe  
0.948295 0.948605 0.500522 Fe  
0.783245 0.027712 0.622697 Fe  
0.907678 0.153038 0.122873 Fe  
0.029772 0.278236 0.622301 Fe  
0.158497 0.403351 0.120945 Fe  
0.284747 0.528055 0.622558 Fe



0.406995 0.651943 0.122839 Fe  
0.531187 0.778477 0.621867 Fe  
0.661545 0.903236 0.119487 Fe  
0.027033 0.783801 0.622054 Fe  
0.156177 0.910196 0.123809 Fe  
0.402727 0.159185 0.120564 Fe  
0.526813 0.284024 0.621980 Fe  
0.653657 0.406883 0.122441 Fe  
0.472462 0.715329 0.378022 Fe  
0.600006 0.840875 0.877622 Fe  
0.722657 0.966977 0.380305 Fe  
0.972885 0.216658 0.378386 Fe  
0.224110 0.466993 0.379292 Fe  
0.717198 0.470548 0.376030 Fe  
0.840023 0.594982 0.875759 Fe  
0.965099 0.723424 0.379105 Fe  
0.094978 0.847021 0.878297 Fe  
0.218057 0.976683 0.379684 Fe  
0.342404 0.095831 0.876927 Fe  
0.465026 0.222809 0.378972 Fe  
0.222552 0.963292 0.870934 Fe  
0.470297 0.217057 0.871127 Fe  
0.595185 0.339340 0.371249 Fe  
0.721123 0.463571 0.872048 Fe  
0.848482 0.591331 0.371318 Fe  
0.969415 0.713882 0.869838 Fe  
0.094803 0.840477 0.372984 Fe  
0.461306 0.721114 0.870959 Fe  
0.589321 0.848183 0.372724 Fe  
0.837626 0.095133 0.371009 Fe  
0.963533 0.220053 0.871349 Fe  
0.090045 0.346885 0.372286 Fe  
0.213964 0.472793 0.871296 Fe  
0.339079 0.594744 0.372718 Fe  
0.789347 0.531830 0.130312 Fe  
0.909419 0.654156 0.625992 Fe  
0.032502 0.775645 0.130158 Fe  
0.161594 0.904813 0.626925 Fe  
0.286770 0.028716 0.128810 Fe  
0.408364 0.151508 0.627834 Fe  
0.532803 0.280414 0.127170 Fe  
0.661130 0.404272 0.628595 Fe  
0.029133 0.286216 0.128833 Fe  
0.155259 0.409094 0.626010 Fe  
0.276659 0.536577 0.128162 Fe  
0.403080 0.660986 0.627846 Fe  
0.529844 0.788073 0.130653 Fe  
0.654290 0.909797 0.626690 Fe

0.903212 0.160365 0.627662 Fe  
0.002125 0.001220 0.000757 N  
0.122189 0.127314 0.500394 N  
0.250568 0.249809 -0.000005 N  
0.375502 0.376036 0.500990 N  
0.502252 0.499538 0.999837 N  
0.624188 0.624203 0.498778 N  
0.750043 0.748512 0.997391 N  
0.876154 0.876134 0.502178 N  
0.437792 0.941337 0.252033 N  
0.560256 0.063478 0.749416 N  
0.685567 0.189524 0.250588 N  
0.811602 0.309948 0.749061 N  
0.939023 0.436639 0.250532 N  
0.064470 0.562555 0.747573 N  
0.188302 0.686973 0.252066 N  
0.310385 0.812955 0.747139 N  
0.063333 0.564063 0.000727 V  
0.438908 0.934718 0.499575 V  
0.875437 0.875477 0.256093 V  
0.189003 0.685119 0.000078 V  
0.438774 0.936503 0.999280 V  
0.989857 0.489650 0.748118 V  
0.260103 0.764220 0.253499 V  
0.938198 0.919024 0.005411 V  
0.579148 0.575372 0.006614 V  
0.701616 0.695564 0.498331 V  
0.271070 0.037018 0.624263 V  
0.771796 0.528532 0.620203 V  
0.898756 0.654614 0.119381 V  
0.346614 0.593628 0.875825 V  
0.848510 0.089393 0.875214 V  
0.098525 0.334521 0.877570 V  
0.591592 0.342188 0.875352 V  
0.344598 0.094626 0.370727 V  
0.713758 0.969405 0.867971 V  
0.774788 0.036917 0.127960 V

**x/16 = 0.1875:**

V12 Fe52 N8  
1.0  
11.421543 0.011554 6.247109  
11.431001 5.696113 -0.006727  
-0.004231 5.697210 6.265431  
Fe N V  
52 8 12

direct

0.374598 0.625162 0.877191 Fe  
0.125003 0.375784 0.124729 Fe  
0.248923 0.001259 -0.000774 Fe  
0.497737 0.253219 0.749071 Fe  
0.751622 0.498312 0.500748 Fe  
-0.000643 0.751547 0.248311 Fe  
0.127202 0.874372 0.624835 Fe  
0.374980 0.124481 0.376054 Fe  
0.623889 0.375327 0.123500 Fe  
0.874279 0.624632 0.875997 Fe  
0.000133 0.249699 0.750959 Fe  
0.499545 0.750754 0.252314 Fe  
0.750375 0.000326 0.000141 Fe  
0.227192 0.520607 0.974803 Fe  
0.481826 0.768267 0.729377 Fe  
0.975826 0.272573 0.228944 Fe  
0.026094 0.725995 0.772521 Fe  
0.519035 0.229267 0.272480 Fe  
0.776419 0.474159 0.023337 Fe  
0.353788 0.644919 0.351095 Fe  
0.851756 0.148668 0.852443 Fe  
0.102648 0.395941 0.603801 Fe  
0.142747 0.857220 0.146973 Fe  
0.396664 0.106940 0.894696 Fe  
0.650184 0.347415 0.647314 Fe  
0.897186 0.601535 0.398623 Fe  
0.933169 0.689629 0.062626 Fe  
0.186282 0.935331 0.819279 Fe  
0.430900 0.187614 0.570844 Fe  
0.679553 0.441193 0.315288 Fe  
0.939289 0.181611 0.059256 Fe  
0.187249 0.432500 0.808533 Fe  
0.554394 0.325634 0.433621 Fe  
0.812084 0.564701 0.189890 Fe  
0.062475 0.817089 0.939509 Fe  
0.312952 0.065829 0.693577 Fe  
0.319690 0.558663 0.685094 Fe  
0.569816 0.807066 0.436443 Fe  
0.814945 0.063998 0.179280 Fe  
0.067735 0.310701 0.933087 Fe  
0.061207 0.811949 0.441118 Fe  
0.301170 0.070930 0.184881 Fe  
0.557567 0.313562 0.941669 Fe  
0.807484 0.562837 0.693317 Fe  
0.817850 0.056110 0.686039 Fe  
0.063882 0.309540 0.435859 Fe  
0.564633 0.807813 0.934884 Fe

0.683907 0.443670 0.812691 Fe  
0.188087 0.940314 0.314765 Fe  
0.435981 0.192961 0.063347 Fe  
0.941832 0.186882 0.557171 Fe  
0.194256 0.433730 0.309982 Fe  
0.000260 0.000240 -0.002484 N  
0.246976 0.250940 0.751519 N  
0.500464 0.499502 0.499771 N  
0.755861 0.743881 0.248657 N  
0.125559 0.125701 0.373263 N  
0.372691 0.376409 0.123517 N  
0.628744 0.621169 0.877416 N  
0.879847 0.872122 0.624730 N  
0.623787 0.872228 0.627570 V  
0.876995 0.127588 0.371583 V  
0.254529 0.492949 0.506799 V  
0.724769 0.029770 0.480484 V  
0.270262 0.986094 0.523493 V  
0.596359 0.895269 0.110120 V  
0.687877 0.934023 0.307033 V  
0.444442 0.676031 0.563636 V  
0.309513 0.561968 0.180999 V  
0.933857 0.692263 0.562434 V  
0.441038 0.688990 0.059309 V  
0.688770 0.942625 0.808616 V

## Cr-alloys

**$x/16 = 0.03125$ :**

Cr4 Fe124 N16

1.0

-0.002434 5.671165 12.463532

-0.000021 5.673498 -12.464600

-11.355112 0.002454 0.001102

Cr Fe N

4 124 16

direct

0.936642 0.561249 0.499559 Cr

0.198505 0.301673 0.750095 Cr

0.872704 0.372488 0.379059 Cr

0.377068 0.377801 0.121343 Cr

0.062780 0.437813 0.499722 Fe

0.062182 0.437942 0.001136 Fe

0.812238 0.687764 0.499858 Fe

0.812041 0.687293 0.000020 Fe  
0.312905 0.187315 0.499344 Fe  
0.312466 0.185955 -0.000405 Fe  
0.562894 0.937818 0.499876 Fe  
0.562467 0.937909 0.000185 Fe  
0.311894 0.686887 0.249779 Fe  
0.312658 0.688394 0.750070 Fe  
0.063267 0.938628 0.249863 Fe  
0.062909 0.937680 0.749987 Fe  
0.563289 0.437329 0.250746 Fe  
0.562144 0.437081 0.750457 Fe  
0.811878 0.186641 0.249141 Fe  
0.811672 0.187252 0.749994 Fe  
0.937675 0.562604 0.000729 Fe  
0.687692 0.812159 0.499978 Fe  
0.687337 0.812074 -0.000028 Fe  
0.187484 0.312750 0.500100 Fe  
0.186266 0.312263 -0.001364 Fe  
0.438154 0.062726 0.499778 Fe  
0.437467 0.062659 0.000338 Fe  
0.186796 0.811685 0.250084 Fe  
0.187349 0.811932 0.749719 Fe  
0.938397 0.063345 0.249887 Fe  
0.938542 0.063292 0.749935 Fe  
0.437501 0.563338 0.250774 Fe  
0.436784 0.561652 0.750271 Fe  
0.687776 0.313096 0.249961 Fe  
0.687835 0.312425 0.749735 Fe  
0.051259 0.448764 0.749817 Fe  
0.050709 0.447868 0.251243 Fe  
0.801028 0.698431 0.750284 Fe  
0.801304 0.699041 0.249845 Fe  
0.302950 0.197552 0.750235 Fe  
0.302060 0.198806 0.249531 Fe  
0.552028 0.949121 0.749353 Fe  
0.551384 0.948525 0.249960 Fe  
0.948732 0.551530 0.748007 Fe  
0.947480 0.551110 0.253242 Fe  
0.697994 0.800798 0.750759 Fe  
0.698350 0.801210 0.249683 Fe  
0.198653 0.301910 0.249649 Fe  
0.449623 0.051222 0.749675 Fe  
0.448478 0.051252 0.250020 Fe  
0.426953 0.573885 0.499657 Fe  
0.427165 0.575752 -0.000922 Fe  
0.174579 0.821498 0.500168 Fe  
0.176460 0.823706 0.000128 Fe  
0.676826 0.324917 0.501074 Fe

0.676336 0.323449 0.000270 Fe  
0.926791 0.073680 0.499505 Fe  
0.926407 0.073654 -0.000113 Fe  
0.323799 0.676626 0.499889 Fe  
0.323536 0.676942 0.000659 Fe  
0.073386 0.926138 0.499624 Fe  
0.073593 0.926336 -0.000017 Fe  
0.574192 0.426938 0.499712 Fe  
0.575198 0.426669 -0.000558 Fe  
0.822277 0.174123 0.500608 Fe  
0.822815 0.176034 0.000477 Fe  
0.127958 0.628436 0.878453 Fe  
0.127922 0.628044 0.379054 Fe  
0.878829 0.879088 0.878417 Fe  
0.878702 0.878770 0.378304 Fe  
0.376512 0.375567 0.878531 Fe  
0.378371 0.378772 0.377764 Fe  
0.628607 0.128668 0.878591 Fe  
0.629033 0.129133 0.377313 Fe  
0.371398 0.871664 0.878750 Fe  
0.371357 0.871501 0.378006 Fe  
0.123755 0.122361 0.877664 Fe  
0.122093 0.122609 0.378384 Fe  
0.620641 0.620643 0.878753 Fe  
0.621286 0.621044 0.378226 Fe  
0.871584 0.372211 0.878572 Fe  
0.628857 0.128905 0.620749 Fe  
0.628231 0.128833 0.121700 Fe  
0.377700 0.376649 0.622591 Fe  
0.878790 0.878873 0.621568 Fe  
0.878752 0.878975 0.121670 Fe  
0.128718 0.627985 0.620565 Fe  
0.127387 0.627988 0.122614 Fe  
0.872002 0.371475 0.620573 Fe  
0.871196 0.371903 0.123058 Fe  
0.621080 0.621116 0.621775 Fe  
0.620330 0.620458 0.122621 Fe  
0.123576 0.122311 0.622484 Fe  
0.122605 0.122882 0.120570 Fe  
0.371771 0.871745 0.621237 Fe  
0.371330 0.871379 0.121722 Fe  
0.503589 0.753193 0.628371 Fe  
0.503381 0.753439 0.128703 Fe  
0.253292 0.002651 0.627898 Fe  
0.253512 0.003377 0.128480 Fe  
0.753836 0.504240 0.628377 Fe  
0.753403 0.503295 0.128843 Fe  
0.001951 0.253823 0.627368 Fe

0.003510 0.253549 0.128335 Fe  
0.747312 0.995755 0.628572 Fe  
0.746807 0.996245 0.128273 Fe  
0.496554 0.247072 0.628209 Fe  
0.495816 0.247104 0.128857 Fe  
0.995898 0.746358 0.628296 Fe  
0.996320 0.747542 0.128189 Fe  
0.246626 0.498338 0.627474 Fe  
0.247736 0.495259 0.128404 Fe  
0.001862 0.254631 0.371722 Fe  
0.001543 0.253475 0.872235 Fe  
0.754728 0.503648 0.371145 Fe  
0.754421 0.502923 0.871583 Fe  
0.253499 0.001670 0.372016 Fe  
0.253548 0.003150 0.871432 Fe  
0.503331 0.753542 0.371616 Fe  
0.503041 0.754442 0.871464 Fe  
0.246280 0.496683 0.371643 Fe  
0.246306 0.498096 0.872381 Fe  
0.996128 0.746527 0.371577 Fe  
0.996549 0.746625 0.871768 Fe  
0.497592 0.246884 0.371256 Fe  
0.496291 0.246069 0.871536 Fe  
0.746983 0.996259 0.371296 Fe  
0.746785 0.996512 0.871580 Fe  
0.251443 0.751197 0.499583 N  
0.249146 0.749427 0.000545 N  
0.000558 0.000612 0.499600 N  
0.000021 0.000174 0.000427 N  
0.499443 0.499408 0.499740 N  
0.497163 0.497286 0.002523 N  
0.751849 0.251902 0.497425 N  
0.750396 0.250603 0.000397 N  
0.625301 0.875303 0.249925 N  
0.625005 0.874972 0.749892 N  
0.374247 0.124206 0.250770 N  
0.375635 0.123770 0.749418 N  
0.875397 0.625923 0.248339 N  
0.875080 0.625263 0.751232 N  
0.124739 0.374939 0.250034 N  
0.125774 0.374250 0.749785 N

**x/16 = 0.0625:**

Cr4 Fe60 N8

1.0

11.330472 0.001283 6.253917

11.329569 5.665382 0.002821

0.001933 5.664606 6.251614  
Cr Fe N  
4 60 8  
direct  
0.758606 0.493963 0.501145 Cr  
0.229276 0.520696 0.977281 Cr  
0.422092 0.691993 0.563436 Cr  
0.307954 0.064818 0.190660 Cr  
0.377327 0.621827 0.876402 Fe  
0.624599 0.873830 0.625194 Fe  
0.874530 0.126526 0.375417 Fe  
0.123604 0.377385 0.124406 Fe  
0.250881 -0.001584 -0.001184 Fe  
0.498593 0.250963 0.751310 Fe  
0.000224 0.749515 0.249078 Fe  
0.120647 0.877143 0.624989 Fe  
0.377195 0.123734 0.376300 Fe  
0.625836 0.374164 0.126057 Fe  
0.874925 0.625627 0.875043 Fe  
0.003029 0.247362 0.751112 Fe  
0.248664 0.501054 0.500352 Fe  
0.499560 0.750263 0.249297 Fe  
0.749945 -0.000101 -0.000064 Fe  
0.484882 0.763754 0.722907 Fe  
0.725718 0.024502 0.476908 Fe  
0.972197 0.276452 0.231742 Fe  
0.019410 0.730930 0.768648 Fe  
0.273005 0.977403 0.523223 Fe  
0.522612 0.228408 0.271866 Fe  
0.772608 0.477108 0.022235 Fe  
0.351245 0.647537 0.351261 Fe  
0.603243 0.896494 0.103959 Fe  
0.854564 0.146276 0.852805 Fe  
0.103192 0.396440 0.603591 Fe  
0.146400 0.853694 0.147106 Fe  
0.396090 0.103440 0.896976 Fe  
0.652218 0.352288 0.644133 Fe  
0.896740 0.600944 0.398157 Fe  
0.933311 0.690068 0.064704 Fe  
0.185584 0.935577 0.818516 Fe  
0.430553 0.191180 0.566950 Fe  
0.677310 0.445293 0.317537 Fe  
0.689675 0.931551 0.311281 Fe  
0.940623 0.181498 0.061591 Fe  
0.187162 0.435535 0.810264 Fe  
0.558847 0.320025 0.439842 Fe  
0.809278 0.570357 0.186638 Fe  
0.061666 0.815955 0.937160 Fe



0.312791 0.064995 0.690204 Fe  
0.313649 0.563472 0.684101 Fe  
0.564270 0.813106 0.428696 Fe  
0.818852 0.059966 0.181951 Fe  
0.070418 0.308123 0.935835 Fe  
0.055319 0.816139 0.441422 Fe  
0.560219 0.312549 0.941715 Fe  
0.809258 0.563232 0.694981 Fe  
0.813029 0.058437 0.686087 Fe  
0.069130 0.304934 0.433269 Fe  
0.314117 0.557841 0.186072 Fe  
0.563665 0.807792 0.938073 Fe  
0.687028 0.441629 0.815731 Fe  
0.934267 0.693906 0.563129 Fe  
0.188215 0.941173 0.313285 Fe  
0.436977 0.189623 0.066378 Fe  
0.442939 0.685529 0.057450 Fe  
0.691173 0.936290 0.808321 Fe  
0.947687 0.181135 0.558491 Fe  
0.192290 0.434823 0.310123 Fe  
0.000797 -0.000417 -0.000075 N  
0.249943 0.249285 0.750685 N  
0.498222 0.502808 0.502732 N  
0.750477 0.750082 0.250680 N  
0.129898 0.122696 0.370513 N  
0.373808 0.375405 0.123817 N  
0.624580 0.626117 0.876225 N  
0.871367 0.877444 0.623881 N

**x/16 = 0.09375:**

Cr12 Fe116 N16

1.0

-5.659695 -11.313939 0.006031

5.660132 -11.314158 0.003795

-0.002557 5.651648 12.514391

Cr Fe N

12 116 16

direct

0.653249 0.656387 0.122735 Cr

0.842892 0.844251 0.872577 Cr

0.096928 0.587056 0.375505 Cr

0.223879 0.720855 0.396533 Cr

0.589798 0.583337 0.352199 Cr

0.781303 0.785674 0.146230 Cr

0.564112 0.810700 0.504705 Cr

0.189490 0.441011 0.492402 Cr

0.432801 0.188790 0.997764 Cr

0.118247 0.385747 0.256706 Cr  
0.625329 0.870632 0.251982 Cr  
0.124504 0.379564 0.750756 Cr  
0.904056 0.907218 0.125717 Fe  
0.405799 0.406960 0.124976 Fe  
0.156685 0.156499 0.125717 Fe  
0.031145 0.031504 0.625330 Fe  
0.783672 0.780709 0.625712 Fe  
0.532011 0.531452 0.626630 Fe  
0.282308 0.280107 0.623481 Fe  
0.532344 0.029471 0.126191 Fe  
0.282857 0.781186 0.125220 Fe  
0.029641 0.531567 0.123785 Fe  
0.781042 0.281774 0.125166 Fe  
0.655890 0.156302 0.623715 Fe  
0.403158 0.908944 0.626819 Fe  
0.156709 0.656579 0.624834 Fe  
0.906081 0.405015 0.623658 Fe  
0.593259 0.593678 0.874213 Fe  
0.344550 0.345193 0.874961 Fe  
0.093588 0.094914 0.875893 Fe  
0.969354 0.966609 0.374711 Fe  
0.719778 0.716201 0.375669 Fe  
0.468215 0.469320 0.373794 Fe  
0.219257 0.218349 0.375313 Fe  
0.468319 0.968604 0.872693 Fe  
0.217320 0.718894 0.875169 Fe  
0.969146 0.469083 0.876228 Fe  
0.719533 0.216924 0.874967 Fe  
0.593966 0.094435 0.375382 Fe  
0.343300 0.841584 0.374203 Fe  
0.843456 0.344364 0.375572 Fe  
0.149703 0.651514 0.102934 Fe  
0.897089 0.403381 0.101795 Fe  
0.650432 0.150118 0.103396 Fe  
0.401418 0.898450 0.102961 Fe  
0.276080 0.776537 0.605731 Fe  
0.028090 0.526076 0.601814 Fe  
0.775623 0.275649 0.603218 Fe  
0.526511 0.025687 0.602855 Fe  
0.096673 0.604449 0.898431 Fe  
0.850090 0.348511 0.896700 Fe  
0.601719 0.097425 0.895886 Fe  
0.348571 0.849392 0.897628 Fe  
0.971938 0.474396 0.397488 Fe  
0.723765 0.224569 0.396952 Fe  
0.473073 0.972587 0.397749 Fe  
0.840094 0.836140 0.355757 Fe

0.340802 0.338068 0.352347 Fe  
0.089059 0.087696 0.353201 Fe  
0.961985 0.961807 0.853605 Fe  
0.714074 0.714756 0.851999 Fe  
0.462734 0.464064 0.852358 Fe  
0.210847 0.215040 0.852465 Fe  
0.537865 0.538376 0.144353 Fe  
0.283226 0.288036 0.148053 Fe  
0.036830 0.037257 0.147487 Fe  
0.912077 0.911519 0.647841 Fe  
0.662066 0.661371 0.648504 Fe  
0.413463 0.411454 0.647197 Fe  
0.161025 0.162093 0.646600 Fe  
0.189973 0.431655 0.998089 Fe  
0.939470 0.183491 0.000995 Fe  
0.685537 0.935194 0.999098 Fe  
0.438257 0.681780 0.998790 Fe  
0.316014 0.558869 0.502272 Fe  
0.065485 0.307426 0.500828 Fe  
0.814346 0.056961 0.499368 Fe  
0.068080 0.311769 0.001879 Fe  
0.817268 0.062065 0.001843 Fe  
0.565308 0.811641 0.997622 Fe  
0.317704 0.560638 0.000327 Fe  
0.942910 0.184906 0.498948 Fe  
0.692330 0.934398 0.498371 Fe  
0.440182 0.688581 0.502859 Fe  
0.681574 0.437225 0.996911 Fe  
0.182804 0.939736 0.000523 Fe  
0.932002 0.689140 0.999693 Fe  
0.808407 0.566133 0.503667 Fe  
0.557691 0.314637 0.499966 Fe  
0.307813 0.063480 0.500776 Fe  
0.060029 0.814379 0.502761 Fe  
0.061462 0.820102 0.004382 Fe  
0.809811 0.567075 0.997953 Fe  
0.560598 0.316421 0.000453 Fe  
0.312837 0.067197 0.001757 Fe  
0.186519 0.939887 0.499481 Fe  
0.935165 0.693086 0.498225 Fe  
0.685936 0.442614 0.502153 Fe  
0.434883 0.191842 0.498612 Fe  
0.877857 0.620461 0.251564 Fe  
0.625401 0.370568 0.246915 Fe  
0.377255 0.120227 0.250531 Fe  
0.125680 0.870165 0.248243 Fe  
0.003086 0.743316 0.748359 Fe  
0.753551 0.494995 0.752604 Fe

0.501106 0.246412 0.750573 Fe  
0.250600 0.996306 0.750286 Fe  
0.754137 0.498547 0.249160 Fe  
0.504958 0.247509 0.246836 Fe  
0.256903 0.997747 0.250943 Fe  
0.000694 0.748306 0.247278 Fe  
0.881959 0.619543 0.747897 Fe  
0.630960 0.373230 0.751269 Fe  
0.379009 0.126149 0.751405 Fe  
0.129370 0.873875 0.751140 Fe  
0.371237 0.625629 0.246751 Fe  
0.870611 0.126818 0.252058 Fe  
0.494256 0.752609 0.750598 Fe  
0.245710 0.499738 0.748011 Fe  
0.994669 0.252365 0.748874 Fe  
0.743746 0.002071 0.746054 Fe  
0.748161 0.003279 0.251419 Fe  
0.500521 0.754340 0.253854 Fe  
0.248444 0.504073 0.247110 Fe  
0.999740 0.255173 0.251477 Fe  
0.873887 0.129320 0.749971 Fe  
0.620196 0.881214 0.745076 Fe  
0.372881 0.630366 0.750192 Fe  
0.748707 0.751587 0.000369 N  
0.499339 0.498020 0.998381 N  
0.254078 0.248403 0.000571 N  
-0.000021 0.001370 0.000412 N  
0.875061 0.875939 0.501347 N  
0.622803 0.627975 0.498445 N  
0.373949 0.375088 0.499820 N  
0.125166 0.124680 0.499998 N  
0.441446 0.937341 0.250446 N  
0.186282 0.688592 0.251387 N  
0.940365 0.435735 0.249374 N  
0.688317 0.187076 0.250035 N  
0.561309 0.064621 0.749527 N  
0.311662 0.813674 0.751771 N  
0.065489 0.557834 0.749999 N  
0.813183 0.311527 0.749951 N

**$x/16 = 0.125$ :**

Cr4 Fe28 N4

1.0

-0.003474 -5.631764 6.306787

-0.002959 5.627390 6.302765

-5.628392 0.001929 -6.301824

Cr Fe N

4 28 4

direct

0.116182 0.617904 -0.004409 Cr  
0.102450 0.603463 0.498558 Cr  
0.514946 0.749963 0.248474 Cr  
0.506805 0.253637 0.253768 Cr  
0.374458 0.874518 -0.002653 Fe  
0.873900 0.373344 0.001355 Fe  
0.878336 0.874491 0.502380 Fe  
0.371908 0.373772 0.500295 Fe  
0.625476 0.124583 -0.000368 Fe  
0.624252 0.625008 0.500572 Fe  
0.124880 0.124658 0.500479 Fe  
0.603385 0.104188 0.502756 Fe  
0.391595 0.889587 0.487690 Fe  
0.903247 0.398541 0.510711 Fe  
0.347028 0.357422 -0.003082 Fe  
0.857237 0.852064 0.000598 Fe  
0.148288 0.146492 0.001520 Fe  
0.648329 0.643726 -0.004089 Fe  
0.499040 0.255635 0.756737 Fe  
0.000735 0.757297 0.755823 Fe  
0.260190 0.507149 0.760030 Fe  
0.754045 -0.002429 0.755719 Fe  
0.743297 0.498374 0.248608 Fe  
0.246507 0.002103 0.240442 Fe  
-0.000713 0.244215 0.247236 Fe  
0.251134 0.504708 0.257838 Fe  
0.747011 0.003783 0.252929 Fe  
0.005261 0.750771 0.257061 Fe  
0.498184 0.751952 0.744983 Fe  
0.988531 0.244282 0.740312 Fe  
0.253417 0.998309 0.747797 Fe  
0.745404 0.492328 0.738064 Fe  
0.000022 0.002713 0.000783 N  
0.502493 0.503739 0.005606 N  
0.741916 0.246075 0.491093 N  
0.250825 0.751632 0.504388 N

**x/16 = 0.15625:**

Cr20 Fe108 N16

1.0

11.262878 -0.003520 -6.304984  
0.003372 -11.263311 -6.305357  
-5.626468 5.626447 -6.292637

Cr Fe N

20 108 16

direct

0.378667 0.623155 0.754468 Cr  
 0.877475 0.625818 0.252816 Cr  
 0.371826 0.124256 0.750860 Cr  
 0.751169 0.003741 0.499067 Cr  
 0.248761 0.002090 0.002045 Cr  
 0.820980 0.822949 0.146231 Cr  
 0.697823 0.197989 0.896527 Cr  
 0.929112 0.927410 0.353897 Cr  
 0.076555 0.071382 0.144271 Cr  
 0.803609 0.298855 0.602709 Cr  
 0.061656 0.056013 0.875852 Cr  
 0.185347 0.687747 0.126468 Cr  
 0.247105 0.505827 0.251519 Cr  
 0.751762 0.002739 0.257171 Cr  
 0.439641 0.438004 0.122072 Cr  
 0.175686 0.685626 0.617978 Cr  
 0.935979 0.423190 0.118346 Cr  
 0.874618 0.121970 0.498128 Cr  
 0.251907 0.001406 0.247846 Cr  
 0.128124 0.370976 -0.002312 Cr  
 0.249690 0.000103 0.501044 Fe  
 0.625433 0.873975 0.249748 Fe  
 0.750960 0.499687 0.499064 Fe  
 -0.003205 0.746939 -0.001785 Fe  
 0.125137 0.379086 0.252037 Fe  
 0.501567 0.250358 0.000249 Fe  
 0.873820 0.126736 0.751197 Fe  
 0.499145 0.748842 0.501369 Fe  
 0.000979 0.251249 0.500219 Fe  
 0.248968 0.502098 0.000740 Fe  
 0.626321 0.375215 0.751842 Fe  
 0.375060 0.128425 0.250750 Fe  
 0.749578 -0.001446 -0.001007 Fe  
 0.125053 0.871598 0.750877 Fe  
 0.874867 0.623748 0.749754 Fe  
 0.125464 0.878202 0.251120 Fe  
 0.498031 0.751511 0.001674 Fe  
 0.251514 0.499154 0.500480 Fe  
 0.626847 0.374322 0.251886 Fe  
 0.002128 0.244329 -0.001779 Fe  
 0.623623 0.875679 0.748846 Fe  
 -0.002132 0.753027 0.497612 Fe  
 0.125316 0.373689 0.749451 Fe  
 0.375998 0.627400 0.254109 Fe  
 0.750128 0.498565 -0.001000 Fe  
 0.499741 0.249500 0.498826 Fe  
 0.877771 0.123762 0.249855 Fe

0.073351 0.073237 0.649381 Fe  
0.449989 0.947968 0.398072 Fe  
0.571531 0.573459 0.649665 Fe  
0.200686 0.695214 0.895644 Fe  
0.948742 0.454124 0.392512 Fe  
0.323564 0.326841 0.147239 Fe  
0.181910 0.170245 0.856225 Fe  
0.550726 0.052224 0.603503 Fe  
0.675761 0.676838 0.853665 Fe  
0.301045 0.803764 0.105177 Fe  
0.050282 0.550528 0.602837 Fe  
0.427796 0.428999 0.352561 Fe  
0.801924 0.299581 0.105816 Fe  
0.198596 0.700397 0.395656 Fe  
0.574379 0.574633 0.147391 Fe  
0.697070 0.197778 0.394082 Fe  
0.948937 0.446707 0.893413 Fe  
0.323176 0.321261 0.649495 Fe  
0.443323 0.951305 0.896208 Fe  
0.821968 0.824948 0.644167 Fe  
0.301307 0.796991 0.607405 Fe  
0.678997 0.676008 0.352261 Fe  
0.046434 0.548667 0.105618 Fe  
0.426931 0.430523 0.850533 Fe  
0.179795 0.179202 0.354960 Fe  
0.550224 0.051951 0.102943 Fe  
0.925907 0.924472 0.851848 Fe  
0.434988 0.935055 0.627757 Fe  
0.562315 0.561328 0.882511 Fe  
0.810970 0.814124 0.378760 Fe  
0.936404 0.435510 0.625520 Fe  
0.311143 0.313282 0.377983 Fe  
0.687731 0.184024 0.127188 Fe  
0.120856 0.874003 -0.001252 Fe  
0.497064 0.754674 0.752468 Fe  
0.623177 0.377457 0.003133 Fe  
0.872650 0.631109 0.502909 Fe  
-0.000240 0.251611 0.753545 Fe  
0.370586 0.127905 0.496581 Fe  
0.377552 0.622535 0.008299 Fe  
0.752826 0.496574 0.750241 Fe  
0.876869 0.120258 -0.002379 Fe  
0.128370 0.372659 0.498713 Fe  
0.504198 0.247782 0.248890 Fe  
0.249705 0.991912 0.745536 Fe  
0.628276 0.872131 0.499695 Fe  
0.005543 0.751359 0.248957 Fe  
0.187248 0.188754 0.620047 Fe

0.563733 0.063558 0.370372 Fe  
0.688472 0.688436 0.621439 Fe  
0.936701 0.935776 0.118462 Fe  
0.312440 0.814268 0.872662 Fe  
0.069132 0.568128 0.375372 Fe  
0.816092 0.313920 0.876879 Fe  
0.561277 0.560293 0.378066 Fe  
0.685878 0.185758 0.625390 Fe  
0.312077 0.316994 0.884690 Fe  
0.063584 0.064191 0.379557 Fe  
0.435837 0.938526 0.130055 Fe  
0.809399 0.809674 0.874140 Fe  
0.245956 0.501889 0.746670 Fe  
0.624084 0.376771 0.500765 Fe  
0.746493 0.003103 0.749521 Fe  
0.000214 0.252155 0.250001 Fe  
0.371972 0.130869 0.003397 Fe  
0.122957 0.879210 0.502593 Fe  
0.496479 0.754599 0.251874 Fe  
0.870013 0.623959 -0.003360 Fe  
0.502199 0.249049 0.750533 Fe  
0.001742 0.745602 0.747621 Fe  
0.624633 0.872372 -0.001909 Fe  
0.376286 0.619890 0.498234 Fe  
0.753875 0.495247 0.247257 Fe  
0.312727 0.815921 0.373315 Fe  
0.686957 0.687631 0.120028 Fe  
0.815752 0.311788 0.371361 Fe  
0.065315 0.563691 0.873737 Fe  
0.438239 0.435590 0.618119 Fe  
0.186961 0.193286 0.123313 Fe  
0.562392 0.063235 0.871784 Fe  
0.939879 0.941287 0.624181 Fe  
0.374687 0.873735 0.749319 N  
0.748516 0.749833 0.500377 N  
0.875146 0.372946 0.747958 N  
0.126419 0.624534 0.244773 N  
0.498888 0.499317 0.003820 N  
0.250757 0.251388 0.501669 N  
0.625481 0.122879 0.248723 N  
0.001754 -0.001989 -0.001088 N  
0.501372 0.499222 0.501159 N  
0.877734 0.374932 0.250104 N  
0.000290 0.002373 0.500133 N  
0.249024 0.253606 -0.000102 N  
0.624143 0.126675 0.751790 N  
0.372808 0.878416 0.250944 N  
0.749360 0.750777 0.000228 N



0.125692 0.625880 0.747556 N

**x/16 = 0.1875:**

Cr12 Fe52 N8

1.0

11.243278 5.604181 -0.002571

-11.251465 5.620550 -0.006517

0.001007 -0.004964 6.317998

Cr Fe N

12 52 8

direct

0.750732 0.751864 0.250936 Cr

0.377446 0.627465 0.238196 Cr

0.244868 0.241842 0.739256 Cr

0.126665 0.374707 0.798148 Cr

0.246583 0.749307 0.703265 Cr

0.500252 0.500483 0.295546 Cr

0.183344 0.064102 -0.011151 Cr

0.064688 0.686705 0.010102 Cr

0.070386 0.193769 0.496689 Cr

0.194189 0.068213 0.512618 Cr

0.441584 0.814689 0.515560 Cr

0.435033 0.310128 0.501123 Cr

-0.000068 0.498609 0.253035 Fe

0.251892 0.250797 0.244638 Fe

0.499243 -0.001627 0.249012 Fe

0.124300 0.877343 0.253372 Fe

0.626627 0.377546 0.247551 Fe

0.873193 0.122705 0.249130 Fe

0.751361 0.750683 0.747889 Fe

-0.000245 0.499525 0.745219 Fe

0.499391 0.001929 0.750036 Fe

0.127144 0.874421 0.743632 Fe

0.371132 0.622479 0.753284 Fe

0.625489 0.374108 0.751423 Fe

0.876759 0.127120 0.753318 Fe

0.621260 0.868688 0.207619 Fe

0.871848 0.626554 0.208319 Fe

0.129592 0.378967 0.210460 Fe

0.373319 0.124332 0.202214 Fe

0.627469 0.876643 0.794677 Fe

0.878311 0.625937 0.791292 Fe

0.376153 0.124018 0.792380 Fe

-0.004119 -0.000271 0.706269 Fe

0.494693 0.495739 0.712993 Fe

0.749971 0.249201 0.707964 Fe

-0.000259 -0.000950 0.294757 Fe

0.258337 0.751899 0.290611 Fe  
0.749826 0.249714 0.291457 Fe  
0.688901 0.066714 0.003269 Fe  
0.943840 0.817922 -0.004893 Fe  
0.184606 0.565796 0.001615 Fe  
0.439092 0.316299 -0.002215 Fe  
0.935006 0.311919 0.006000 Fe  
0.433230 0.811960 -0.005752 Fe  
0.685119 0.561647 -0.009450 Fe  
0.315459 0.435932 -0.000457 Fe  
0.567611 0.189401 0.003152 Fe  
0.816932 0.939035 -0.001406 Fe  
0.560486 0.682169 -0.013469 Fe  
0.813213 0.434214 -0.000452 Fe  
0.060967 0.182617 0.010679 Fe  
0.308506 0.932655 0.002926 Fe  
0.313421 0.942241 0.496349 Fe  
0.558949 0.689297 0.514361 Fe  
0.813849 0.442305 0.501462 Fe  
0.308381 0.435601 0.494952 Fe  
0.558259 0.187494 0.497578 Fe  
0.807505 0.937880 0.503038 Fe  
0.058946 0.686411 0.486130 Fe  
0.689678 0.562725 0.510767 Fe  
0.941571 0.312632 0.496364 Fe  
0.938714 0.808820 0.506453 Fe  
0.187691 0.559478 0.496032 Fe  
0.684967 0.057995 0.500284 Fe  
0.000966 -0.000936 0.000532 N  
0.247800 0.750198 -0.004946 N  
0.502319 0.500152 0.005976 N  
0.750894 0.250446 -0.000726 N  
0.375044 0.128043 0.495968 N  
0.621783 0.873829 0.500250 N  
0.873604 0.624111 0.499517 N  
0.124301 0.373615 0.507271 N

## Mn-alloys

$x/16 = 0.03125$ :

Mn4 Fe124 N16

1.0

5.676927 5.678545 12.458863

-5.680814 -5.679239 12.460958

5.681976 -5.679707 -12.460639

Fe Mn N

124 4 16

direct

0.062530 0.812685 0.750122 Fe  
0.063846 0.312531 0.250192 Fe  
0.562786 0.312654 0.749994 Fe  
0.312397 0.062309 0.749847 Fe  
0.312331 0.562634 0.250240 Fe  
0.812538 0.562508 0.750083 Fe  
0.561816 0.811600 0.250141 Fe  
0.812778 0.064716 0.249537 Fe  
0.312088 0.562000 0.749156 Fe  
0.312114 0.062742 0.250015 Fe  
0.812740 0.062849 0.750720 Fe  
0.562088 0.812219 0.748862 Fe  
0.562382 0.312791 0.249986 Fe  
0.063052 0.313028 0.750747 Fe  
0.812724 0.563101 0.250165 Fe  
0.063683 0.812023 0.249842 Fe  
0.937407 0.687528 0.749925 Fe  
0.937972 0.186363 0.250124 Fe  
0.437403 0.187563 0.750286 Fe  
0.187576 0.937577 0.750228 Fe  
0.187411 0.437579 0.249952 Fe  
0.687542 0.437339 0.749871 Fe  
0.437446 0.687040 0.249655 Fe  
0.187588 0.437365 0.750245 Fe  
0.187316 0.937630 0.249896 Fe  
0.687621 0.937610 0.750167 Fe  
0.437947 0.688179 0.751220 Fe  
0.438498 0.186744 0.250164 Fe  
0.936840 0.186856 0.748695 Fe  
0.686200 0.437834 0.249977 Fe  
0.936880 0.687247 0.249971 Fe  
0.801334 0.801529 0.500242 Fe  
0.801466 0.301098 -0.000437 Fe  
0.301346 0.301088 0.499713 Fe  
0.052032 0.051797 0.500672 Fe  
0.051707 0.551078 0.000211 Fe  
0.551087 0.551351 0.499903 Fe  
0.300811 0.801170 -0.000716 Fe  
0.550957 0.051753 -0.000368 Fe  
0.698499 0.698793 0.500014 Fe  
0.698375 0.198254 -0.000684 Fe  
0.198905 0.198542 0.500039 Fe  
0.947652 0.949657 0.500044 Fe  
0.948759 0.448672 -0.000021 Fe  
0.448855 0.448900 0.500300 Fe

0.198455 0.698411 -0.000520 Fe  
0.451856 0.948943 0.002862 Fe  
0.176272 0.676185 0.499882 Fe  
0.176387 0.176435 0.000310 Fe  
0.676347 0.173023 0.497136 Fe  
0.426118 0.926131 0.499727 Fe  
0.926969 0.426960 0.501453 Fe  
0.675111 0.677610 0.001020 Fe  
0.926546 0.926076 -0.000076 Fe  
0.074639 0.574557 0.501399 Fe  
0.074062 0.073908 0.000535 Fe  
0.573495 0.073521 0.500077 Fe  
0.323710 0.823255 0.499667 Fe  
0.323907 0.324030 0.000511 Fe  
0.823513 0.324098 0.500268 Fe  
0.572981 0.573291 -0.000180 Fe  
0.823100 0.823099 -0.001489 Fe  
0.622030 0.621838 0.243756 Fe  
0.621414 0.121390 0.742797 Fe  
0.121424 0.121678 0.243112 Fe  
0.871630 0.371334 0.742843 Fe  
0.371468 0.371250 0.243035 Fe  
0.121012 0.621181 0.742261 Fe  
0.371309 0.871596 0.743223 Fe  
0.622953 0.378272 0.000962 Fe  
0.621463 0.878601 0.500233 Fe  
0.121283 0.878339 -0.000206 Fe  
0.871537 0.628290 -0.000079 Fe  
0.873941 0.129984 0.500711 Fe  
0.371631 0.128106 0.000281 Fe  
0.121917 0.378408 0.500268 Fe  
0.371237 0.628571 0.500131 Fe  
0.878786 0.122620 0.001318 Fe  
0.878424 0.622130 0.500756 Fe  
0.378151 0.621772 -0.000331 Fe  
0.128659 0.371315 0.000028 Fe  
0.126827 0.871637 0.498848 Fe  
0.628276 0.872009 -0.003192 Fe  
0.378442 0.121460 0.499865 Fe  
0.628602 0.371434 0.500049 Fe  
0.878407 0.878675 0.757232 Fe  
0.378494 0.378182 0.756480 Fe  
0.128499 0.128526 0.757048 Fe  
0.128269 0.628565 0.257098 Fe  
0.628615 0.628436 0.757299 Fe  
0.378158 0.878431 0.256735 Fe  
0.629820 0.130531 0.257122 Fe  
0.996003 0.496073 0.242565 Fe

0.996638 0.996680 0.743282 Fe  
0.494002 0.995253 0.242873 Fe  
0.246435 0.746696 0.242806 Fe  
0.246098 0.246014 0.742497 Fe  
0.746856 0.246896 0.242801 Fe  
0.496887 0.496952 0.743484 Fe  
0.746658 0.746467 0.742884 Fe  
0.996528 0.253691 -0.000195 Fe  
0.996764 0.753711 0.500369 Fe  
0.494177 0.751408 -0.001028 Fe  
0.246067 0.503810 0.000340 Fe  
0.246625 0.003506 0.499888 Fe  
0.746289 0.003480 -0.000495 Fe  
0.497041 0.253299 0.500015 Fe  
0.746628 0.503562 0.500339 Fe  
0.253593 0.996552 0.000044 Fe  
0.253995 0.496672 0.500051 Fe  
0.753227 0.496967 -0.000043 Fe  
0.503438 0.246087 -0.000112 Fe  
0.503715 0.746550 0.499951 Fe  
0.003696 0.746676 -0.000192 Fe  
0.752517 0.995204 0.501070 Fe  
0.003501 0.246624 0.500093 Fe  
0.253598 0.753782 0.757291 Fe  
0.254092 0.253835 0.257400 Fe  
0.753482 0.253270 0.756378 Fe  
0.503438 0.003361 0.756737 Fe  
0.503508 0.503677 0.257692 Fe  
0.003404 0.503756 0.757115 Fe  
0.753300 0.751337 0.257565 Fe  
0.003111 0.003157 0.257061 Fe  
0.689057 0.936661 0.249726 Mn  
0.426908 0.427345 0.000242 Mn  
0.868649 0.871608 0.240164 Mn  
0.880063 0.379502 0.259660 Mn  
-0.001992 0.498207 0.496069 N  
-0.000234 0.000478 0.000173 N  
0.499819 0.000011 0.500113 N  
0.249413 0.750844 0.500280 N  
0.250137 0.249597 -0.000288 N  
0.750010 0.249468 0.499832 N  
0.500035 0.499005 0.000055 N  
0.750536 0.750794 0.001784 N  
0.375627 0.374948 0.500515 N  
0.375475 0.875507 0.000481 N  
0.875347 0.875283 0.500318 N  
0.625034 0.624839 0.500030 N  
0.624882 0.125281 -0.000242 N

0.125183 0.125123 0.500155 N  
0.874421 0.374856 -0.000720 N  
0.124852 0.625017 -0.000071 N

**x/16 = 0.0625:**

Mn4 Fe60 N8

1.0

5.673446 -5.664884 6.234053

-5.671907 -5.663268 6.234125

0.000847 -5.670868 -6.240296

Fe Mn N

60 4 8

direct

0.437113 0.437631 0.625093 Fe

0.186321 0.187350 0.125194 Fe

0.937520 0.937144 0.624886 Fe

0.688152 0.687418 0.124465 Fe

0.563178 0.062523 0.376650 Fe

0.312486 0.812379 0.874851 Fe

0.062630 0.562389 0.374930 Fe

0.812259 0.312607 0.874955 Fe

0.311767 0.313030 0.873263 Fe

0.062794 0.062650 0.374968 Fe

0.812373 0.812639 0.875091 Fe

0.562954 0.561469 0.374935 Fe

0.187777 0.687319 0.124934 Fe

0.937282 0.437465 0.624211 Fe

0.689473 0.187819 0.124637 Fe

0.175602 0.676019 0.645838 Fe

0.926275 0.426031 0.146079 Fe

0.676759 0.177184 0.646027 Fe

0.426664 0.925669 0.145320 Fe

0.073081 0.573857 0.853085 Fe

0.574073 0.073321 0.851251 Fe

0.324038 0.824406 0.354188 Fe

0.426106 0.426730 0.146075 Fe

0.176099 0.175357 0.646691 Fe

0.926681 0.926133 0.146673 Fe

0.675709 0.676458 0.648460 Fe

0.322591 0.324881 0.354446 Fe

0.072934 0.073920 0.853874 Fe

0.825425 0.822841 0.353866 Fe

0.573790 0.573817 0.854473 Fe

0.931378 0.689052 0.621749 Fe

0.682410 0.439993 0.120908 Fe

0.432657 0.191611 0.620706 Fe

0.182004 0.938504 0.121999 Fe

0.811575 0.567936 0.378014 Fe  
 0.560013 0.317747 0.879228 Fe  
 0.312086 0.069144 0.374235 Fe  
 0.060425 0.817295 0.878317 Fe  
 0.939741 0.182027 0.121389 Fe  
 0.691895 0.932984 0.620974 Fe  
 0.439245 0.682574 0.123145 Fe  
 0.188760 0.432163 0.622057 Fe  
 0.317490 0.561080 0.878111 Fe  
 0.068450 0.310693 0.378380 Fe  
 0.817970 0.060995 0.877653 Fe  
 0.183358 0.438122 0.121693 Fe  
 0.932022 0.189039 0.622178 Fe  
 0.682455 0.938562 0.122743 Fe  
 0.431598 0.687148 0.622388 Fe  
 0.060508 0.317716 0.878006 Fe  
 0.811406 0.067126 0.377690 Fe  
 0.560994 0.817173 0.882044 Fe  
 0.310791 0.568178 0.378017 Fe  
 0.186387 0.931493 0.623390 Fe  
 0.939720 0.682228 0.121550 Fe  
 0.688443 0.432397 0.622821 Fe  
 0.566251 0.310920 0.376666 Fe  
 0.315913 0.060959 0.880916 Fe  
 0.068334 0.810709 0.377667 Fe  
 0.817941 0.560805 0.878618 Fe  
 0.436929 0.937553 0.625425 Mn  
 0.823559 0.323094 0.354847 Mn  
 0.570388 0.810329 0.377332 Mn  
 0.440081 0.180499 0.120965 Mn  
 0.250678 0.248512 0.500061 N  
 -0.000007 -0.000232 0.000213 N  
 0.746216 0.751047 0.498273 N  
 0.499760 0.500518 0.000641 N  
 0.499306 0.003022 0.000751 N  
 0.250316 0.750539 0.500248 N  
 0.000980 0.499610 0.000387 N  
 0.749670 0.250680 0.498194 N

**x/16 = 0.09375:**

Mn12 Fe116 N16  
 1.0  
 11.331272 -5.664518 6.250767  
 -11.330395 -5.664371 6.249341  
 -0.000365 -5.668249 -6.253550  
 Fe Mn N  
 116 12 16

direct

0.187039 0.687894 0.623887 Fe  
0.437417 0.436838 0.625976 Fe  
0.687770 0.187376 0.624719 Fe  
0.186056 0.187197 0.123458 Fe  
0.938095 0.938086 0.622743 Fe  
0.684394 0.687835 0.127934 Fe  
0.937369 0.438263 0.124257 Fe  
0.188692 0.438133 0.375182 Fe  
0.439170 0.187203 0.375640 Fe  
0.684531 0.935813 0.371937 Fe  
0.188407 0.937775 0.875382 Fe  
0.937668 0.687213 0.374693 Fe  
0.439230 0.688819 0.877930 Fe  
0.686922 0.437085 0.875415 Fe  
0.937783 0.188359 0.875123 Fe  
0.061583 0.562580 0.875632 Fe  
0.311935 0.312264 0.874157 Fe  
0.563323 0.063063 0.873052 Fe  
0.061253 0.062245 0.375101 Fe  
0.311959 0.812434 0.377218 Fe  
0.562793 0.561939 0.375161 Fe  
0.812107 0.312592 0.375035 Fe  
0.062817 0.312050 0.626102 Fe  
0.312601 0.062083 0.626349 Fe  
0.061499 0.812397 0.123896 Fe  
0.812068 0.563456 0.626030 Fe  
0.311710 0.560281 0.127153 Fe  
0.563363 0.312537 0.125190 Fe  
0.814036 0.062941 0.123140 Fe  
0.051624 0.801603 0.646232 Fe  
0.300760 0.550625 0.647220 Fe  
0.552251 0.301459 0.647161 Fe  
0.051576 0.301584 0.145890 Fe  
0.801909 0.052025 0.645231 Fe  
0.302189 0.049247 0.145709 Fe  
0.800853 0.552253 0.146910 Fe  
0.946999 0.700217 0.852098 Fe  
0.198448 0.447778 0.853610 Fe  
0.449046 0.198007 0.851964 Fe  
0.701172 0.948002 0.848607 Fe  
0.198180 0.947445 0.353090 Fe  
0.448903 0.698379 0.355993 Fe  
0.698292 0.448465 0.353828 Fe  
0.175161 0.676583 0.147253 Fe  
0.426495 0.425431 0.147026 Fe  
0.677589 0.177280 0.146387 Fe  
0.924762 0.924867 0.143775 Fe



0.427104 0.927264 0.647819 Fe  
0.677502 0.677942 0.651701 Fe  
0.926202 0.427500 0.647905 Fe  
0.074109 0.574118 0.353862 Fe  
0.323315 0.324149 0.355006 Fe  
0.573708 0.072970 0.350885 Fe  
0.073555 0.073316 0.853039 Fe  
0.822370 0.822812 0.352404 Fe  
0.324313 0.825172 0.853686 Fe  
0.572912 0.572535 0.855102 Fe  
0.823501 0.324317 0.853249 Fe  
0.872744 0.750529 0.616777 Fe  
0.122390 0.500678 0.623536 Fe  
0.372586 0.250156 0.622082 Fe  
0.872441 0.251157 0.121857 Fe  
0.622115 0.001439 0.618982 Fe  
0.122217 -0.000020 0.122912 Fe  
0.621330 0.500333 0.122162 Fe  
0.749564 0.628531 0.378057 Fe  
0.750544 0.128792 0.878210 Fe  
0.497243 0.875564 0.385568 Fe  
0.002989 0.880360 0.875670 Fe  
0.499312 0.377873 0.879929 Fe  
0.749774 0.372039 0.122169 Fe  
0.000728 0.121621 0.121130 Fe  
0.248736 0.869910 0.122509 Fe  
0.752061 0.873456 0.614212 Fe  
0.497692 0.619492 0.127127 Fe  
-0.000372 0.621334 0.622258 Fe  
0.250256 0.371341 0.621894 Fe  
0.500406 0.121857 0.620071 Fe  
0.128154 0.750257 0.878215 Fe  
0.378672 0.501167 0.877911 Fe  
0.629012 0.250368 0.878056 Fe  
0.127917 0.250927 0.377555 Fe  
0.880853 0.002498 0.875785 Fe  
0.377283 -0.000028 0.380303 Fe  
0.626334 0.747759 0.379029 Fe  
0.877972 0.500338 0.378669 Fe  
0.996277 0.624873 0.121844 Fe  
0.247069 0.374061 0.122158 Fe  
0.498484 0.126250 0.119623 Fe  
0.996020 0.124285 0.622950 Fe  
0.747183 0.876329 0.120016 Fe  
0.246458 0.874792 0.622348 Fe  
0.746508 0.375486 0.622014 Fe  
0.875090 0.503773 0.878587 Fe  
0.124776 0.253067 0.879122 Fe

0.375880 0.004964 0.876588 Fe  
0.874308 0.002301 0.376794 Fe  
0.623797 0.751793 0.880180 Fe  
0.125039 0.753485 0.378168 Fe  
0.375214 0.503386 0.378437 Fe  
0.625025 0.253252 0.378812 Fe  
0.875305 0.247604 0.621459 Fe  
0.125224 0.996234 0.620949 Fe  
0.372560 0.745048 0.623920 Fe  
0.873394 0.745280 0.124532 Fe  
0.624328 0.497124 0.622623 Fe  
0.125045 0.496095 0.122214 Fe  
0.629880 0.000093 0.114496 Fe  
0.254768 0.625390 0.378004 Fe  
0.502889 0.374574 0.377952 Fe  
0.753111 0.125072 0.377213 Fe  
0.253298 0.124579 0.878772 Fe  
0.002617 0.874529 0.377544 Fe  
0.505643 0.877376 0.873579 Fe  
0.751458 0.622889 0.881809 Fe  
0.003694 0.375683 0.878504 Fe  
0.439836 0.936018 0.125766 Mn  
0.813018 0.812937 0.872306 Mn  
0.563268 0.813002 0.626158 Mn  
0.546692 0.803957 0.142818 Mn  
0.947819 0.198234 0.354368 Mn  
0.176910 0.177041 0.646033 Mn  
0.368556 0.744867 0.126192 Mn  
0.001003 0.380063 0.379347 Mn  
0.251287 0.130025 0.376440 Mn  
0.250840 0.629836 0.880356 Mn  
0.495323 0.624339 0.623260 Mn  
0.373963 0.243873 0.122376 Mn  
0.000239 0.498200 0.498344 N  
0.249302 0.247371 0.498550 N  
0.499681 -0.000381 0.497719 N  
0.000533 0.000051 0.001168 N  
0.748645 0.749478 0.500541 N  
0.251593 0.748745 -0.000399 N  
0.498937 0.499762 0.001261 N  
0.751114 0.250677 0.000158 N  
0.125429 0.374725 -0.000029 N  
0.375382 0.126470 0.001770 N  
0.624118 0.874602 -0.000615 N  
0.124621 0.875284 0.499619 N  
0.875037 0.625597 -0.000444 N  
0.376942 0.624828 0.504324 N  
0.624685 0.375423 0.500412 N

0.875543 0.125482 0.498222 N

**x/16 = 0.125:**

Mn4 Fe28 N4

1.0

-0.000755 -5.664182 6.244639

0.002456 5.669551 6.249549

-5.667247 -0.004290 -6.247870

Fe Mn N

28 4 4

direct

0.374411 0.875523 -0.001636 Fe

0.876408 0.874257 0.500108 Fe

0.374909 0.375366 0.499926 Fe

0.122570 0.624845 -0.000821 Fe

0.625457 0.124379 -0.000163 Fe

0.625616 0.624475 0.501721 Fe

0.124516 0.124028 0.498592 Fe

0.602142 0.104634 0.501063 Fe

0.102641 0.602113 0.498836 Fe

0.396621 0.897997 0.501600 Fe

0.896192 0.396809 0.498789 Fe

0.354135 0.351794 -0.000563 Fe

0.146987 0.147336 0.001317 Fe

0.647981 0.646220 -0.001509 Fe

0.495966 0.256122 0.756190 Fe

0.000941 0.756801 0.756492 Fe

0.256304 0.499472 0.756679 Fe

0.754976 -0.003211 0.752917 Fe

0.742148 0.499718 0.244952 Fe

0.244855 -0.000760 0.243753 Fe

0.000480 0.242042 0.245278 Fe

0.254454 0.509496 0.257787 Fe

0.747552 0.005398 0.256508 Fe

0.008866 0.753573 0.259171 Fe

0.507364 0.249409 0.257448 Fe

0.491339 0.749759 0.742489 Fe

0.249092 0.993454 0.743658 Fe

0.749383 0.495076 0.740966 Fe

0.875153 0.375189 0.000029 Mn

0.854126 0.855042 -0.000061 Mn

0.499394 0.741177 0.240737 Mn

0.993304 0.249404 0.739984 Mn

-0.001162 -0.000273 -0.000386 N

0.500828 0.503832 0.004153 N

0.755402 0.250445 0.506141 N

0.248646 0.749059 0.497855 N

**x/16 = 0.15625:**

Mn20 Fe108 N16

1.0

5.656855 5.660729 -12.520295

5.664254 5.660849 12.523728

5.654746 -5.654980 0.001671

Fe Mn N

108 20 16

direct

0.311323 0.935632 0.749934 Fe

0.563991 0.188995 0.254290 Fe

0.813089 0.937165 0.251027 Fe

0.063685 0.187441 0.749069 Fe

0.312178 0.437525 0.249906 Fe

0.562715 0.687333 0.749870 Fe

0.812543 0.437974 0.745837 Fe

0.061821 0.685796 0.250839 Fe

0.563462 0.189947 0.746102 Fe

0.062784 0.186461 0.251196 Fe

0.312073 0.437242 0.750231 Fe

0.813176 0.936790 0.748195 Fe

0.313500 0.937366 0.250985 Fe

0.438389 0.812885 0.752461 Fe

0.936579 0.812118 0.250036 Fe

0.186857 0.062536 0.750214 Fe

0.436381 0.312573 0.249638 Fe

0.687036 0.563412 0.750155 Fe

0.937975 0.313542 0.752059 Fe

0.187055 0.561966 0.250426 Fe

0.687698 0.061452 0.754317 Fe

0.187794 0.063633 0.250473 Fe

0.436915 0.313518 0.751422 Fe

0.687007 0.563441 0.250829 Fe

0.937586 0.812453 0.750150 Fe

0.187528 0.561991 0.749229 Fe

0.439341 0.814197 0.246860 Fe

0.198555 0.800704 0.501377 Fe

0.447214 0.052283 0.003009 Fe

0.698766 0.799978 0.000250 Fe

0.948690 0.050378 0.500387 Fe

0.199485 0.302343 -0.000503 Fe

0.448994 0.551419 0.499667 Fe

0.948881 0.551811 -0.000238 Fe

0.301901 0.698067 0.499643 Fe

0.801725 0.699093 -0.000194 Fe

0.051906 0.948078 0.500828 Fe

0.550554 0.448841 0.501311 Fe  
0.801075 0.197925 0.494686 Fe  
0.050714 0.448358 -0.000133 Fe  
0.323173 0.176848 0.499268 Fe  
0.572488 0.427001 0.000298 Fe  
0.073643 0.426510 0.499062 Fe  
0.574617 0.926640 0.497158 Fe  
0.823322 0.677080 0.500327 Fe  
0.073801 0.926146 -0.000849 Fe  
0.426944 0.073631 0.498086 Fe  
0.676282 0.325709 0.001569 Fe  
0.927719 0.071400 0.000434 Fe  
0.176444 0.322571 0.500575 Fe  
0.425967 0.574018 0.000684 Fe  
0.676660 0.823472 0.499192 Fe  
0.925645 0.573263 0.500221 Fe  
0.175711 0.822154 -0.001054 Fe  
0.250253 0.750365 0.244057 Fe  
0.750052 0.750851 0.742680 Fe  
0.000852 -0.000764 0.243062 Fe  
0.249612 0.249671 0.742384 Fe  
0.499771 0.497549 0.243268 Fe  
0.747379 0.248580 0.242430 Fe  
-0.000089 0.498427 0.742881 Fe  
0.370497 0.873391 0.000190 Fe  
0.623908 0.120375 0.500944 Fe  
0.872459 0.871412 0.499968 Fe  
0.120624 0.121884 0.000336 Fe  
0.370700 0.371335 0.500052 Fe  
0.621975 0.619990 -0.001302 Fe  
0.867878 0.373705 -0.003012 Fe  
0.122085 0.620159 0.498220 Fe  
0.623819 0.134300 -0.003747 Fe  
0.882473 0.375011 0.502719 Fe  
0.127951 0.128280 0.499971 Fe  
0.378037 0.379264 0.000352 Fe  
0.629915 0.627644 0.502257 Fe  
0.878438 0.879461 -0.000230 Fe  
0.379804 0.878291 0.499884 Fe  
0.252579 0.749740 0.755613 Fe  
0.497383 0.002272 0.257907 Fe  
0.751813 0.750333 0.257350 Fe  
0.000280 0.000318 0.756963 Fe  
0.248732 0.250666 0.257503 Fe  
0.499419 0.499808 0.757656 Fe  
0.000349 0.500137 0.256796 Fe  
0.374658 0.124713 0.243297 Fe  
0.624172 0.377018 0.745105 Fe

0.374938 0.624885 0.742497 Fe  
0.627673 0.874094 0.242810 Fe  
0.874872 0.626249 0.244089 Fe  
0.124671 0.876630 0.742082 Fe  
0.497048 0.246481 0.001025 Fe  
0.743515 0.499534 0.501838 Fe  
0.244846 0.495742 -0.000285 Fe  
0.495536 0.748025 0.502194 Fe  
0.752011 0.992971 -0.004035 Fe  
0.995881 0.746929 0.002499 Fe  
0.247724 0.997202 0.501193 Fe  
0.002809 0.753726 0.498682 Fe  
0.253183 0.502260 0.499475 Fe  
0.504507 0.753519 -0.002685 Fe  
0.754112 0.004503 0.501021 Fe  
0.252045 0.001655 0.001570 Fe  
0.500596 0.255098 0.501175 Fe  
0.621802 0.377099 0.256497 Fe  
0.878234 0.121137 0.257399 Fe  
0.123949 0.374439 0.756775 Fe  
0.372610 0.625159 0.257262 Fe  
0.627127 0.874486 0.755891 Fe  
0.873531 0.625446 0.756552 Fe  
0.811050 0.434976 0.256310 Mn  
0.562095 0.687238 0.250284 Mn  
0.062525 0.687244 0.749977 Mn  
0.687694 0.062363 0.240802 Mn  
0.934308 0.310483 0.245865 Mn  
0.700705 0.304517 0.504030 Mn  
0.554939 0.951955 -0.003732 Mn  
0.301366 0.198264 0.000712 Mn  
0.826585 0.178621 0.000611 Mn  
0.323329 0.677071 0.000056 Mn  
0.499075 0.002961 0.743617 Mn  
0.129792 0.627747 0.001366 Mn  
0.750075 0.249032 0.754429 Mn  
0.875824 0.125962 0.743894 Mn  
0.123512 0.373207 0.242638 Mn  
0.995377 0.246206 0.499582 Mn  
0.754727 0.504904 0.000121 Mn  
0.005026 0.250030 -0.001354 Mn  
0.376401 0.123394 0.758803 Mn  
0.125164 0.874735 0.259018 Mn  
0.501178 0.000386 0.503182 N  
0.750185 0.248954 -0.000860 N  
0.001506 -0.000512 0.000088 N  
0.249676 0.249795 0.500044 N  
0.499464 0.500519 0.001107 N

0.749824 0.750052 0.499332 N  
-0.000228 0.499874 0.499441 N  
0.248185 0.747313 -0.000879 N  
0.625489 0.374473 0.499742 N  
0.873318 0.623400 0.000518 N  
0.122461 0.373233 0.004403 N  
0.375628 0.624874 0.499066 N  
0.625516 0.877102 0.000990 N  
0.877170 0.126802 0.500613 N  
0.125487 0.874823 0.496991 N  
0.373210 0.125441 -0.002693 N

**x/16 = 0.1875:**

Mn12 Fe52 N8

1.0

-5.663830 -5.656866 6.268673

5.658600 5.662297 6.268881

-5.650893 5.649159 -6.263917

Fe Mn N

52 12 8

direct

0.622563 0.874047 0.250967 Fe

0.127168 0.877884 0.751011 Fe

0.622001 0.372309 0.749302 Fe

0.375862 0.126579 0.251321 Fe

0.874058 0.622017 0.248448 Fe

0.373832 0.624770 0.750421 Fe

0.375021 0.625415 0.251101 Fe

0.876998 0.628676 0.753849 Fe

0.873837 0.124451 0.246443 Fe

0.374992 0.124028 0.748799 Fe

0.125233 0.874914 0.247692 Fe

0.624468 0.373462 0.249423 Fe

0.125127 0.374795 0.750194 Fe

0.853956 0.854792 0.501469 Fe

0.353972 0.855134 0.001529 Fe

0.853561 0.351409 0.000395 Fe

0.646572 0.647209 0.500442 Fe

0.147919 0.648205 0.001624 Fe

0.147212 0.146577 0.500025 Fe

0.853640 0.353681 0.500344 Fe

0.352227 0.351615 -0.000182 Fe

0.353524 0.853630 0.500109 Fe

0.647175 0.146788 0.500440 Fe

0.149277 0.150111 0.001195 Fe

0.147337 0.647224 0.498468 Fe

0.643282 0.642250 -0.000378 Fe

0.377770 0.878352 0.256667 Fe  
0.377276 0.378057 0.756405 Fe  
0.874735 0.376703 0.256331 Fe  
0.880690 0.123954 0.001476 Fe  
0.377968 0.120921 0.498965 Fe  
0.377574 0.621093 0.000633 Fe  
0.619492 0.376880 -0.000592 Fe  
0.126184 0.881717 0.000794 Fe  
0.619737 0.876304 0.497847 Fe  
0.622936 0.621670 0.244178 Fe  
0.121150 0.622290 0.745096 Fe  
0.123055 0.121271 0.243082 Fe  
0.620324 0.122779 0.742086 Fe  
0.382797 0.380577 0.258874 Fe  
0.377206 0.877446 0.755899 Fe  
0.873766 0.619619 0.000444 Fe  
0.380348 0.623787 0.502307 Fe  
0.378876 0.121436 -0.000211 Fe  
0.880270 0.124014 0.498064 Fe  
0.617845 0.872163 0.002658 Fe  
0.119777 0.877347 0.497907 Fe  
0.124696 0.382668 -0.000009 Fe  
0.625129 0.380528 0.502621 Fe  
0.622059 0.121722 0.243779 Fe  
0.122725 0.120954 0.740422 Fe  
0.122521 0.625268 0.241767 Fe  
0.126174 0.375666 0.250251 Mn  
0.874841 0.123024 0.749409 Mn  
0.631183 0.878367 0.753903 Mn  
0.351797 0.353780 0.497900 Mn  
0.645077 0.143461 -0.001695 Mn  
0.849095 0.852615 -0.004192 Mn  
0.882133 0.878859 0.756834 Mn  
0.880800 0.621854 0.502501 Mn  
0.117996 0.378514 0.500715 Mn  
0.880551 0.383254 0.759667 Mn  
0.875110 0.874891 0.252655 Mn  
0.622383 0.619624 0.746386 Mn  
0.501395 0.000297 0.501112 N  
-0.003359 -0.002493 -0.003237 N  
0.000576 0.500422 0.499526 N  
0.497947 0.497805 0.000204 N  
0.501411 0.501823 0.504494 N  
-0.001694 0.498563 -0.003238 N  
-0.002680 -0.001458 0.495503 N  
0.501540 -0.000357 -0.000634 N



## Co-alloys

**x/16 = 0.03125:**

Fe124 Co4 N16

1.0

-5.696293 5.696293 6.231106

5.696293 5.696293 -6.231106

-17.088879 0.000000 -6.231106

Co Fe N

4 124 16

direct

0.968750 0.531250 0.187500 Co

0.985337 0.014663 0.676442 Co

0.973240 0.783945 0.189296 Co

0.401759 0.341055 0.560704 Co

0.218750 0.281250 0.687500 Fe

0.093750 0.406250 0.437500 Fe

0.843750 0.656250 0.937500 Fe

0.718750 0.781250 0.687500 Fe

0.593750 0.906250 0.437500 Fe

0.468750 0.031250 0.187500 Fe

0.343750 0.156250 0.937500 Fe

0.406250 0.593750 0.562500 Fe

0.281250 0.718750 0.312500 Fe

0.156250 0.843750 0.062500 Fe

0.031250 0.968750 0.812500 Fe

0.906250 0.093750 0.562500 Fe

0.781250 0.218750 0.312500 Fe

0.656250 0.343750 0.062500 Fe

0.531250 0.468750 0.812500 Fe

0.031250 0.468750 0.812500 Fe

0.906250 0.593750 0.562500 Fe

0.781250 0.718750 0.312500 Fe

0.656250 0.843750 0.062500 Fe

0.531250 0.968750 0.812500 Fe

0.406250 0.093750 0.562500 Fe

0.281250 0.218750 0.312500 Fe

0.156250 0.343750 0.062500 Fe

0.218750 0.781250 0.687500 Fe

0.093750 0.906250 0.437500 Fe

0.968750 0.031250 0.187500 Fe

0.843750 0.156250 0.937500 Fe

0.718750 0.281250 0.687500 Fe

0.593750 0.406250 0.437500 Fe

0.468750 0.531250 0.187500 Fe

0.343750 0.656250 0.937500 Fe

0.264663 0.235337 0.823558 Fe  
0.139663 0.360337 0.573558 Fe  
0.014663 0.485337 0.323558 Fe  
0.889663 0.610337 0.073558 Fe  
0.764663 0.735337 0.823558 Fe  
0.639663 0.860337 0.573558 Fe  
0.514663 0.985337 0.323558 Fe  
0.389663 0.110337 0.073558 Fe  
0.110337 0.389663 0.926442 Fe  
0.985337 0.514663 0.676442 Fe  
0.860337 0.639663 0.426442 Fe  
0.735337 0.764663 0.176442 Fe  
0.610337 0.889663 0.926442 Fe  
0.485337 0.014663 0.676442 Fe  
0.360337 0.139663 0.426442 Fe  
0.235337 0.264663 0.176442 Fe  
0.639663 0.360337 0.573558 Fe  
0.514663 0.485337 0.323558 Fe  
0.389663 0.610337 0.073558 Fe  
0.264663 0.735337 0.823558 Fe  
0.139663 0.860337 0.573558 Fe  
0.014663 0.985337 0.323558 Fe  
0.889663 0.110337 0.073558 Fe  
0.764663 0.235337 0.823558 Fe  
0.485337 0.514663 0.676442 Fe  
0.360337 0.639663 0.426442 Fe  
0.235337 0.764663 0.176442 Fe  
0.110337 0.889663 0.926442 Fe  
0.860337 0.139663 0.426442 Fe  
0.735337 0.264663 0.176442 Fe  
0.610337 0.389663 0.926442 Fe  
0.348241 0.408945 0.939296 Fe  
0.223241 0.533945 0.689296 Fe  
0.098241 0.658945 0.439296 Fe  
0.848241 0.908945 0.939296 Fe  
0.723241 0.033945 0.689296 Fe  
0.598241 0.158945 0.439296 Fe  
0.473241 0.283945 0.189296 Fe  
0.591055 0.651759 0.939296 Fe  
0.466055 0.776759 0.689296 Fe  
0.341055 0.901759 0.439296 Fe  
0.216055 0.026759 0.189296 Fe  
0.091055 0.151759 0.939296 Fe  
0.966055 0.276759 0.689296 Fe  
0.841055 0.401759 0.439296 Fe  
0.716055 0.526759 0.189296 Fe  
0.783945 0.973241 0.810704 Fe  
0.658945 0.098241 0.560704 Fe

0.533945 0.223241 0.310704 Fe  
0.408945 0.348241 0.060704 Fe  
0.283945 0.473241 0.810704 Fe  
0.158945 0.598241 0.560704 Fe  
0.033945 0.723241 0.310704 Fe  
0.908945 0.848241 0.060704 Fe  
0.026759 0.216055 0.810704 Fe  
0.901759 0.341055 0.560704 Fe  
0.776759 0.466055 0.310704 Fe  
0.651759 0.591055 0.060704 Fe  
0.526759 0.716055 0.810704 Fe  
0.401759 0.841055 0.560704 Fe  
0.276759 0.966055 0.310704 Fe  
0.151759 0.091055 0.060704 Fe  
0.723241 0.533945 0.689296 Fe  
0.598241 0.658945 0.439296 Fe  
0.473241 0.783945 0.189296 Fe  
0.348241 0.908945 0.939296 Fe  
0.223241 0.033945 0.689296 Fe  
0.098241 0.158945 0.439296 Fe  
0.973241 0.283945 0.189296 Fe  
0.848241 0.408945 0.939296 Fe  
0.966055 0.776759 0.689296 Fe  
0.841055 0.901759 0.439296 Fe  
0.716055 0.026759 0.189296 Fe  
0.591055 0.151759 0.939296 Fe  
0.466055 0.276759 0.689296 Fe  
0.341055 0.401759 0.439296 Fe  
0.216055 0.526759 0.189296 Fe  
0.091055 0.651759 0.939296 Fe  
0.158945 0.098241 0.560704 Fe  
0.033945 0.223241 0.310704 Fe  
0.908945 0.348241 0.060704 Fe  
0.783945 0.473241 0.810704 Fe  
0.658945 0.598241 0.560704 Fe  
0.533945 0.723241 0.310704 Fe  
0.408945 0.848241 0.060704 Fe  
0.283945 0.973241 0.810704 Fe  
0.276759 0.466055 0.310704 Fe  
0.151759 0.591055 0.060704 Fe  
0.026759 0.716055 0.810704 Fe  
0.901759 0.841055 0.560704 Fe  
0.776759 0.966055 0.310704 Fe  
0.651759 0.091055 0.060704 Fe  
0.526759 0.216055 0.810704 Fe  
0.375000 0.625000 0.750000 N  
0.250000 0.750000 0.500000 N  
0.125000 0.875000 0.250000 N

0.000000 -0.000000 0.000000 N  
0.875000 0.125000 0.750000 N  
0.750000 0.250000 0.500000 N  
0.625000 0.375000 0.250000 N  
0.500000 0.500000 -0.000000 N  
0.750000 0.750000 0.500000 N  
0.625000 0.875000 0.250000 N  
0.500000 -0.000000 0.000000 N  
0.375000 0.125000 0.750000 N  
0.250000 0.250000 0.500000 N  
0.125000 0.375000 0.250000 N  
-0.000000 0.500000 -0.000000 N  
0.875000 0.625000 0.750000 N

**x/16 = 0.0625:**

Fe60 Co4 N8  
1.0  
11.359116 0.008162 6.222923  
11.360782 5.672849 0.004417  
0.000517 5.676637 6.229446  
Co Fe N  
4 60 8  
direct  
0.750263 -0.000869 0.002477 Co  
0.271716 0.978362 0.522294 Co  
0.433152 0.189160 0.566010 Co  
0.814963 0.057899 0.684512 Co  
0.375310 0.624566 0.875680 Fe  
0.625455 0.874755 0.625815 Fe  
0.874380 0.125562 0.375139 Fe  
0.124871 0.375073 0.124538 Fe  
0.250547 -0.000326 -0.000381 Fe  
0.500180 0.250079 0.748939 Fe  
0.749947 0.499654 0.500461 Fe  
0.000314 0.749670 0.250522 Fe  
0.125318 0.875628 0.624341 Fe  
0.373986 0.124951 0.375385 Fe  
0.625436 0.374448 0.125251 Fe  
0.875489 0.624656 0.875081 Fe  
0.000693 0.249074 0.749055 Fe  
0.249817 0.500272 0.499914 Fe  
0.499036 0.751020 0.250923 Fe  
0.227474 0.522020 0.977514 Fe  
0.477916 0.772108 0.728727 Fe  
0.726482 0.023326 0.477484 Fe  
0.976982 0.272696 0.227254 Fe  
0.022087 0.728107 0.771985 Fe

0.520734 0.228437 0.273011 Fe  
0.772621 0.477530 0.022418 Fe  
0.352624 0.647201 0.353087 Fe  
0.603495 0.896613 0.103145 Fe  
0.852569 0.145884 0.853105 Fe  
0.102652 0.397580 0.602830 Fe  
0.146794 0.853271 0.147713 Fe  
0.398127 0.102385 0.897419 Fe  
0.647670 0.351932 0.647472 Fe  
0.897503 0.602428 0.397069 Fe  
0.931237 0.690648 0.066592 Fe  
0.184149 0.938024 0.817102 Fe  
0.681763 0.439857 0.317647 Fe  
0.687859 0.933648 0.309082 Fe  
0.939902 0.181576 0.060858 Fe  
0.191180 0.430370 0.809683 Fe  
0.439503 0.682729 0.562333 Fe  
0.560015 0.318468 0.438858 Fe  
0.810264 0.568072 0.189224 Fe  
0.059036 0.819000 0.938385 Fe  
0.312521 0.066631 0.688836 Fe  
0.317760 0.560822 0.682638 Fe  
0.567649 0.810189 0.435067 Fe  
0.816822 0.060809 0.182188 Fe  
0.067974 0.310170 0.932342 Fe  
0.056127 0.815809 0.442909 Fe  
0.305608 0.065867 0.191307 Fe  
0.558932 0.311936 0.942684 Fe  
0.807282 0.563989 0.692730 Fe  
0.063025 0.307838 0.434679 Fe  
0.314239 0.557334 0.186276 Fe  
0.565008 0.806895 0.936040 Fe  
0.685825 0.442108 0.814060 Fe  
0.935519 0.692910 0.564166 Fe  
0.184276 0.944648 0.312855 Fe  
0.437319 0.191472 0.064178 Fe  
0.443079 0.685327 0.058200 Fe  
0.694857 0.935841 0.809393 Fe  
0.942178 0.186088 0.555939 Fe  
0.192112 0.435919 0.307432 Fe  
0.000759 0.000139 -0.000521 N  
0.249734 0.249466 0.750568 N  
0.499971 0.500897 0.500036 N  
0.749405 0.749306 0.251196 N  
0.125410 0.124681 0.374937 N  
0.374391 0.375855 0.124830 N  
0.625172 0.624429 0.875377 N  
0.875533 0.875080 0.623703 N

**x/16 = 0.09375:**

Fe116 Co12 N16

1.0

-5.662467 5.663769 -6.225860

5.663959 -5.666369 -6.229593

-11.338312 -11.342023 -0.001018

Co Fe N

12 116 16

direct

0.999117 0.751013 0.376079 Co

0.251289 0.002388 0.873583 Co

0.249518 0.000628 0.625397 Co

0.148304 0.645644 0.999741 Co

0.103917 0.102606 0.750279 Co

0.397037 0.896867 0.250325 Co

0.626117 0.372075 0.250024 Co

0.250347 0.747668 0.371034 Co

0.124054 0.880154 0.001170 Co

0.370862 0.625600 0.750169 Co

0.751549 0.749701 0.128449 Co

0.872152 0.630195 0.247386 Co

0.000354 0.748606 0.876740 Fe

0.500602 0.250601 0.875113 Fe

0.250260 0.500616 0.624409 Fe

0.499856 0.250258 0.375116 Fe

0.249003 0.500729 0.124479 Fe

0.749760 0.999772 0.625048 Fe

0.751077 0.000557 0.124789 Fe

0.999846 0.749600 0.624964 Fe

0.500933 0.250696 0.624670 Fe

0.249414 0.499281 0.374965 Fe

0.001579 0.750035 0.123206 Fe

0.499819 0.250140 0.124836 Fe

0.248960 0.500690 0.876063 Fe

0.750643 0.000487 0.374975 Fe

0.750218 0.999570 0.874992 Fe

0.749227 0.499503 0.874854 Fe

0.499723 0.749541 0.624829 Fe

0.251299 0.999554 0.374538 Fe

0.750070 0.500407 0.374093 Fe

0.499276 0.750041 0.125600 Fe

0.000567 0.250045 0.625828 Fe

0.999463 0.249321 0.125077 Fe

0.749913 0.499966 0.625311 Fe

0.499552 0.750620 0.374220 Fe

0.250757 0.000540 0.126073 Fe

0.749485 0.499761 0.125266 Fe  
0.500149 0.750194 0.875273 Fe  
0.999793 0.250204 0.374926 Fe  
0.000733 0.249360 0.874317 Fe  
0.647848 0.146886 0.999829 Fe  
0.397521 0.397772 0.749992 Fe  
0.147205 0.647938 0.499192 Fe  
0.647237 0.147060 0.500046 Fe  
0.396167 0.397587 0.250095 Fe  
0.897436 0.896095 0.750389 Fe  
0.898011 0.897058 0.249809 Fe  
0.351480 0.853908 0.999745 Fe  
0.852207 0.352172 0.000075 Fe  
0.602213 0.603418 0.750135 Fe  
0.352137 0.853216 0.500037 Fe  
0.852938 0.353528 0.499858 Fe  
0.603343 0.602059 0.249660 Fe  
0.103515 0.102569 0.250003 Fe  
0.896744 0.396375 0.750179 Fe  
0.396509 0.896338 0.749883 Fe  
0.147208 0.146417 0.499920 Fe  
0.896752 0.398355 0.249819 Fe  
0.147573 0.146835 0.000087 Fe  
0.647185 0.647476 0.499701 Fe  
0.647087 0.646855 0.000379 Fe  
0.102771 0.603000 0.750108 Fe  
0.602112 0.103183 0.749936 Fe  
0.352754 0.352780 0.500090 Fe  
0.101050 0.603370 0.250594 Fe  
0.603987 0.102637 0.249871 Fe  
0.352550 0.352781 0.999759 Fe  
0.852952 0.853153 0.499708 Fe  
0.852872 0.852585 0.000333 Fe  
0.379247 0.624309 0.000238 Fe  
0.879194 0.121691 0.999876 Fe  
0.627419 0.371483 0.749893 Fe  
0.378362 0.622281 0.499380 Fe  
0.878543 0.122668 0.500209 Fe  
0.128720 0.873601 0.750408 Fe  
0.125614 0.867308 0.251375 Fe  
0.498579 0.499279 0.878524 Fe  
0.002345 0.998674 0.878522 Fe  
0.750226 0.250055 0.628436 Fe  
0.500474 0.500488 0.378235 Fe  
0.000019 0.999175 0.378427 Fe  
0.749369 0.250778 0.129244 Fe  
0.250773 0.750549 0.628642 Fe  
0.249864 0.751020 0.128214 Fe

0.499576 0.499736 0.621421 Fe  
0.000646 0.999874 0.622334 Fe  
0.749742 0.251520 0.371016 Fe  
0.499255 0.500183 0.121815 Fe  
0.000799 0.998761 0.121304 Fe  
0.750212 0.249849 0.871514 Fe  
0.251126 0.751887 0.871891 Fe  
0.621172 0.378305 0.000090 Fe  
0.121643 0.877877 0.499568 Fe  
0.622140 0.378752 0.499850 Fe  
0.369918 0.627823 0.250423 Fe  
0.871599 0.126464 0.750123 Fe  
0.871899 0.127305 0.249966 Fe  
0.131005 0.374938 0.750160 Fe  
0.627236 0.871718 0.750171 Fe  
0.377107 0.120797 0.500009 Fe  
0.127350 0.372309 0.249916 Fe  
0.629577 0.873191 0.249280 Fe  
0.376814 0.120824 0.999825 Fe  
0.878686 0.622474 0.499812 Fe  
0.875667 0.618710 0.000058 Fe  
0.250750 0.250394 0.628665 Fe  
0.749841 0.750029 0.628431 Fe  
0.501563 0.001508 0.377726 Fe  
0.249480 0.249585 0.128349 Fe  
0.499056 0.999203 0.878579 Fe  
0.000115 0.502143 0.378154 Fe  
0.998492 0.498448 0.878656 Fe  
0.249223 0.248740 0.371616 Fe  
0.752549 0.750100 0.370668 Fe  
0.500780 0.001154 0.122035 Fe  
0.251026 0.250788 0.871313 Fe  
0.750495 0.750098 0.872063 Fe  
0.498346 0.998734 0.621648 Fe  
0.998256 0.498867 0.121159 Fe  
0.000573 0.500493 0.621927 Fe  
0.872576 0.628450 0.750448 Fe  
0.370789 0.127389 0.749993 Fe  
0.120768 0.377134 0.499805 Fe  
0.373712 0.128984 0.250074 Fe  
0.119067 0.376218 0.000023 Fe  
0.621950 0.878107 0.499477 Fe  
0.622485 0.878389 0.000765 Fe  
0.250168 0.749393 0.750333 N  
0.749989 0.249470 0.750020 N  
0.499927 0.500206 0.499800 N  
0.251021 0.749852 0.250034 N  
0.750352 0.249759 0.250133 N



0.499313 0.500135 0.000046 N  
0.999064 0.000810 0.500305 N  
0.000660 0.999372 0.000134 N  
0.000502 0.499840 0.500557 N  
0.500418 0.999682 0.499528 N  
0.249623 0.249991 0.249984 N  
0.000776 0.499938 0.999889 N  
0.500507 0.999765 0.000711 N  
0.248579 0.250843 0.749853 N  
0.749278 0.750811 0.249414 N  
0.750062 0.749877 0.750070 N

**$x/16 = 0.125$ :**

Fe28 Co4 N4  
1.0  
-0.001442 -5.666521 6.234546  
0.000777 5.664526 6.232725  
-5.669424 -0.000111 -6.233331  
Co Fe N  
4 28 4  
direct  
0.122604 0.124090 0.498716 Co  
0.102795 0.603267 0.500373 Co  
0.501126 0.256411 0.757040 Co  
0.505391 0.249411 0.255258 Co  
0.374259 0.874192 0.998697 Fe  
0.875446 0.375318 0.001020 Fe  
0.874938 0.873884 0.500217 Fe  
0.374767 0.376009 0.500404 Fe  
0.124923 0.624505 0.999898 Fe  
0.624916 0.125387 0.000608 Fe  
0.624936 0.624537 0.499520 Fe  
0.601644 0.102805 0.500103 Fe  
0.397293 0.899596 0.501488 Fe  
0.897264 0.396559 0.500104 Fe  
0.352412 0.351803 0.999285 Fe  
0.852899 0.853099 0.000158 Fe  
0.148219 0.147699 0.001257 Fe  
0.647195 0.646678 0.999383 Fe  
0.000191 0.755264 0.756026 Fe  
0.256004 0.496230 0.754668 Fe  
0.756838 0.000123 0.757471 Fe  
0.742997 0.498459 0.242242 Fe  
0.242301 0.000692 0.244393 Fe  
0.500187 0.744112 0.243464 Fe  
0.999786 0.243117 0.245192 Fe  
0.250996 0.508123 0.257593 Fe

0.751122 0.008815 0.257410 Fe  
0.008571 0.752455 0.258042 Fe  
0.493683 0.751200 0.743243 Fe  
0.994666 0.249823 0.743138 Fe  
0.251206 0.994796 0.742037 Fe  
0.748749 0.492521 0.741691 Fe  
0.999639 0.999675 0.999138 N  
0.500527 0.500504 0.000871 N  
0.749563 0.250162 0.500213 N  
0.249942 0.748673 0.499635 N

**x/16 = 0.15625:**

Fe108 Co20 N16

1.0

-0.001694 5.652694 12.490587

-0.000203 -5.648689 12.488754

11.305238 -0.002493 -6.245724

Co Fe N

20 108 16

direct

0.438256 0.935636 0.500965 Co

0.562555 0.062174 -0.000075 Co

0.624421 0.625024 0.249958 Co

0.191000 0.685475 -0.000707 Co

0.626555 0.625655 0.751405 Co

0.239262 0.738123 0.750697 Co

0.136270 0.635890 0.749918 Co

0.425720 0.426947 -0.000551 Co

0.675327 0.677244 -0.000801 Co

0.052922 0.049922 0.499565 Co

0.160258 0.401242 0.122655 Co

0.154949 0.911275 0.122952 Co

0.399152 0.162168 0.123422 Co

0.221753 0.965556 0.871474 Co

0.345202 0.090780 0.371143 Co

0.969121 0.713392 0.871600 Co

0.719239 0.968838 0.871592 Co

0.032687 0.776730 0.127152 Co

0.403139 0.662217 0.627676 Co

0.902969 0.157968 0.628305 Co

0.812983 0.312048 -0.000399 Fe

0.937247 0.437492 0.499955 Fe

0.061543 0.561820 -0.000070 Fe

0.187911 0.687449 0.500503 Fe

0.312817 0.812947 -0.000848 Fe

0.686789 0.187922 0.499607 Fe

0.125099 0.125537 0.249839 Fe  
0.250793 0.249898 0.750853 Fe  
0.374813 0.375923 0.250375 Fe  
0.499219 0.500413 0.749224 Fe  
0.749357 0.750233 0.750022 Fe  
0.874566 0.875345 0.249778 Fe  
0.000939 -0.001646 0.750357 Fe  
0.688212 0.187660 0.000022 Fe  
0.814353 0.311027 0.500572 Fe  
0.936510 0.437807 -0.000577 Fe  
0.062019 0.562210 0.500584 Fe  
0.310661 0.814000 0.499544 Fe  
0.437591 0.936972 -0.000118 Fe  
0.562471 0.062989 0.500109 Fe  
0.000957 -0.000711 0.249924 Fe  
0.124422 0.124955 0.748452 Fe  
0.249389 0.250034 0.250639 Fe  
0.374642 0.374880 0.751011 Fe  
0.498654 0.499974 0.248691 Fe  
0.749832 0.750260 0.249152 Fe  
0.877242 0.873707 0.750399 Fe  
0.739368 0.238436 0.750202 Fe  
0.864214 0.363836 0.249934 Fe  
0.988214 0.489244 0.750658 Fe  
0.113778 0.613622 0.249963 Fe  
0.365002 0.863642 0.250386 Fe  
0.490490 0.988462 0.751098 Fe  
0.613187 0.114223 0.248530 Fe  
0.637008 0.134973 0.750000 Fe  
0.760995 0.260911 0.249620 Fe  
0.886612 0.384245 0.749355 Fe  
0.011159 0.510177 0.249287 Fe  
0.259553 0.761661 0.247535 Fe  
0.385583 0.886612 0.749681 Fe  
0.510887 0.011340 0.249267 Fe  
0.177225 0.175408 -0.000315 Fe  
0.302067 0.301158 0.500877 Fe  
0.550645 0.552741 0.501424 Fe  
0.801283 0.801301 0.499741 Fe  
0.930961 0.922231 0.001337 Fe  
0.074360 0.072326 -0.001146 Fe  
0.200121 0.197880 0.499902 Fe  
0.323514 0.323383 -0.000478 Fe  
0.447803 0.449307 0.500203 Fe  
0.572754 0.574432 -0.000513 Fe  
0.698358 0.698140 0.500224 Fe  
0.821708 0.825173 -0.001136 Fe  
0.948903 0.948484 0.499741 Fe

0.784095 0.026946 0.621980 Fe  
0.909750 0.151281 0.122048 Fe  
0.035023 0.277732 0.622023 Fe  
0.282784 0.528337 0.622874 Fe  
0.408746 0.653145 0.120298 Fe  
0.532660 0.777836 0.621760 Fe  
0.658842 0.903915 0.121108 Fe  
0.027953 0.783587 0.622115 Fe  
0.278282 0.034495 0.621913 Fe  
0.527063 0.284095 0.622091 Fe  
0.652412 0.410938 0.121448 Fe  
0.776348 0.533689 0.622373 Fe  
0.902641 0.658880 0.121530 Fe  
0.347077 0.591859 0.878912 Fe  
0.472077 0.717235 0.377372 Fe  
0.597149 0.841945 0.878565 Fe  
0.722199 0.966778 0.378129 Fe  
0.848596 0.090331 0.877975 Fe  
0.974430 0.216072 0.378459 Fe  
0.097744 0.341558 0.879372 Fe  
0.221993 0.466397 0.378471 Fe  
0.591093 0.349364 0.878397 Fe  
0.716340 0.473045 0.377426 Fe  
0.840475 0.598793 0.878158 Fe  
0.966359 0.722166 0.377959 Fe  
0.093292 0.845883 0.880294 Fe  
0.217958 0.974207 0.378695 Fe  
0.342872 0.097669 0.880474 Fe  
0.465843 0.222732 0.377638 Fe  
0.472875 0.212514 0.873368 Fe  
0.596174 0.340701 0.372142 Fe  
0.719425 0.466049 0.871357 Fe  
0.844344 0.590480 0.371428 Fe  
0.094998 0.839425 0.370336 Fe  
0.463530 0.721653 0.869324 Fe  
0.588202 0.847266 0.372738 Fe  
0.840286 0.095939 0.372399 Fe  
0.964889 0.220344 0.870055 Fe  
0.088995 0.346369 0.371533 Fe  
0.211691 0.474170 0.873169 Fe  
0.339436 0.597141 0.371627 Fe  
0.782908 0.528759 0.127427 Fe  
0.909852 0.653330 0.630225 Fe  
0.160992 0.903470 0.629620 Fe  
0.285915 0.028959 0.128469 Fe  
0.411098 0.152275 0.628383 Fe  
0.534184 0.278330 0.127227 Fe  
0.661150 0.404243 0.628476 Fe

0.028818 0.285047 0.127100 Fe  
0.153495 0.409764 0.629420 Fe  
0.276447 0.536646 0.126488 Fe  
0.528449 0.783683 0.127653 Fe  
0.654540 0.909963 0.629435 Fe  
0.778894 0.034990 0.127726 Fe  
0.000531 0.000186 0.001136 N  
0.124686 0.125333 0.500382 N  
0.249521 0.250786 0.000521 N  
0.374670 0.375326 0.500061 N  
0.500303 0.498874 -0.000542 N  
0.624930 0.624397 0.499497 N  
0.749913 0.749735 0.001042 N  
0.874973 0.874799 0.499653 N  
0.437547 0.938034 0.249822 N  
0.564049 0.061813 0.751155 N  
0.687774 0.187821 0.250600 N  
0.812680 0.311784 0.749619 N  
0.936788 0.437826 0.249474 N  
0.062273 0.563640 0.750629 N  
0.186658 0.688143 0.249413 N  
0.311481 0.812331 0.749235 N

**x/16 = 0.1875:**

Fe52 Co12 N8

1.0

-5.648402 -5.651109 6.240314

5.646110 5.643631 6.231366

-5.641148 5.646147 -6.238183

Co Fe N

12 52 8

direct

0.117306 0.371031 0.247672 Co

0.370939 0.120097 0.748967 Co

0.625764 0.376513 0.252527 Co

0.856339 0.352956 0.003109 Co

0.647453 0.646552 0.499676 Co

0.853719 0.852364 -0.000238 Co

0.377841 0.877710 0.255307 Co

0.381727 0.378545 0.757154 Co

0.617669 0.377120 -0.006012 Co

0.376081 0.378140 0.257424 Co

0.620311 0.876500 -0.000476 Co

0.124937 0.626759 0.242629 Co

0.625704 0.875338 0.251203 Fe

0.125371 0.874510 0.750201 Fe

0.628197 0.375768 0.751784 Fe

0.373821 0.124022 0.250204 Fe  
0.875434 0.127910 0.752884 Fe  
0.874110 0.621518 0.246303 Fe  
0.373477 0.623280 0.748938 Fe  
0.378917 0.626558 0.251772 Fe  
0.873167 0.626082 0.749364 Fe  
0.873729 0.122938 0.248539 Fe  
0.124514 0.876193 0.249743 Fe  
0.624636 0.872669 0.749166 Fe  
0.126669 0.375396 0.751587 Fe  
0.853967 0.853433 0.500293 Fe  
0.353887 0.852847 0.000607 Fe  
0.352196 0.351696 0.499005 Fe  
0.149037 0.648270 0.001716 Fe  
0.148910 0.147533 0.502087 Fe  
0.643742 0.148584 -0.000663 Fe  
0.853968 0.353880 0.500880 Fe  
0.355149 0.352331 0.001149 Fe  
0.353325 0.852601 0.500306 Fe  
0.647132 0.148873 0.501806 Fe  
0.148391 0.150079 0.003206 Fe  
0.145844 0.644425 0.496115 Fe  
0.648135 0.647211 -0.000525 Fe  
0.880887 0.882432 0.756066 Fe  
0.873260 0.374584 0.255035 Fe  
0.874690 0.119775 -0.000358 Fe  
0.378942 0.121385 0.500159 Fe  
0.378701 0.620852 -0.000012 Fe  
0.878376 0.623145 0.498742 Fe  
0.122363 0.378608 0.499732 Fe  
0.122159 0.879820 0.000037 Fe  
0.623316 0.880288 0.499978 Fe  
0.624373 0.620575 0.242960 Fe  
0.121411 0.621771 0.744468 Fe  
0.123501 0.125542 0.243612 Fe  
0.619212 0.121473 0.746091 Fe  
0.881846 0.382221 0.757368 Fe  
0.378828 0.877125 0.755551 Fe  
0.875716 0.875798 0.255384 Fe  
0.879906 0.622355 0.000723 Fe  
0.373473 0.615508 0.495496 Fe  
0.378826 0.123153 0.001054 Fe  
0.878860 0.123074 0.500888 Fe  
0.122336 0.878134 0.499276 Fe  
0.125025 0.383797 0.005314 Fe  
0.619228 0.378216 0.496984 Fe  
0.622404 0.121770 0.243851 Fe  
0.122449 0.122490 0.745583 Fe

0.618463 0.618926 0.743058 Fe  
0.501570 0.000555 0.501582 N  
-0.001678 -0.001682 -0.002760 N  
0.000489 0.501333 0.501470 N  
0.500484 0.499320 -0.000886 N  
0.499428 0.501093 0.498533 N  
-0.000490 0.499477 0.000536 N  
-0.000679 0.000438 0.499493 N  
0.500809 -0.001578 -0.000416 N

## Ni-alloys

**$x/16 = 0.03125$ :**

Fe124 Ni4 N16

1.0

5.669364 0.003654 -6.237554

5.661936 5.659857 6.227417

5.662183 -16.994682 6.241011

Fe N Ni

124 16 4

direct

0.374121 0.093087 0.530907 Fe

0.875581 0.969012 0.156851 Fe

0.374660 0.342703 0.281227 Fe

0.875455 0.220459 0.906679 Fe

0.377117 0.592625 0.030804 Fe

0.875283 0.467792 0.656152 Fe

0.374868 0.842933 0.781221 Fe

0.872479 0.720445 0.407219 Fe

0.624459 0.405987 0.468767 Fe

0.124915 0.281510 0.093511 Fe

0.625715 0.656557 0.218814 Fe

0.127881 0.529284 0.843109 Fe

0.623216 0.906218 0.969060 Fe

0.125595 0.781173 0.593144 Fe

0.624251 0.157250 0.718565 Fe

0.624489 0.906167 0.468930 Fe

0.123257 0.783116 0.094423 Fe

0.624640 0.156455 0.218435 Fe

0.121199 0.028600 0.843005 Fe

0.626142 0.406369 0.968703 Fe

0.124770 0.281656 0.593936 Fe

0.627461 0.659066 0.719519 Fe

0.126379 0.530123 0.343464 Fe

0.873118 0.220143 0.406709 Fe

0.374922 0.092788 0.031185 Fe  
0.875621 0.469413 0.156385 Fe  
0.375329 0.343138 0.781086 Fe  
0.872266 0.722594 0.905286 Fe  
0.374484 0.593932 0.531004 Fe  
0.874364 0.967682 0.658177 Fe  
0.377660 0.841665 0.281248 Fe  
0.147634 0.890062 0.461984 Fe  
0.646200 0.764329 0.088415 Fe  
0.146808 0.138503 0.213943 Fe  
0.647876 0.013806 0.837865 Fe  
0.147638 0.390648 0.963128 Fe  
0.646360 0.264237 0.588356 Fe  
0.149224 0.637708 0.712886 Fe  
0.646717 0.514678 0.338336 Fe  
0.353586 0.736104 0.411996 Fe  
0.854724 0.612413 0.036330 Fe  
0.352601 0.985088 0.161659 Fe  
0.352899 0.234148 0.911591 Fe  
0.853694 0.110361 0.536901 Fe  
0.354326 0.486142 0.661563 Fe  
0.853169 0.360967 0.286607 Fe  
0.146494 0.389800 0.463266 Fe  
0.646678 0.264148 0.088149 Fe  
0.147699 0.639859 0.213757 Fe  
0.647498 0.515020 0.838451 Fe  
0.146914 0.889330 0.962677 Fe  
0.647279 0.764440 0.588730 Fe  
0.146018 0.138793 0.713619 Fe  
0.645708 0.014278 0.338301 Fe  
0.351119 0.234627 0.411379 Fe  
0.853528 0.110855 0.037026 Fe  
0.352994 0.485078 0.161198 Fe  
0.853719 0.361996 0.787023 Fe  
0.351786 0.735528 0.911686 Fe  
0.853578 0.611043 0.536919 Fe  
0.352291 0.985661 0.661486 Fe  
0.856184 0.862919 0.287545 Fe  
0.622643 0.655028 0.965956 Fe  
0.121005 0.030820 0.091459 Fe  
0.617104 0.908240 0.716796 Fe  
0.122749 0.279517 0.840944 Fe  
0.621220 0.154868 0.466064 Fe  
0.121258 0.530699 0.590922 Fe  
0.622079 0.405942 0.216292 Fe  
0.124409 0.900522 0.221229 Fe  
0.618945 0.778864 0.845347 Fe  
0.123191 0.151506 0.968951 Fe



0.623124 0.026272 0.594492 Fe  
0.122249 0.401044 0.719332 Fe  
0.622044 0.276438 0.344416 Fe  
0.121548 0.652691 0.468530 Fe  
0.622466 0.526891 0.094512 Fe  
0.377316 0.223120 0.155474 Fe  
0.873837 0.102400 0.781697 Fe  
0.380009 0.471756 0.905173 Fe  
0.877516 0.348202 0.530538 Fe  
0.378701 0.723177 0.655305 Fe  
0.879692 0.599989 0.281591 Fe  
0.377370 0.971487 0.404562 Fe  
0.876578 0.849086 0.030669 Fe  
0.378264 0.844704 0.533565 Fe  
0.878560 0.719581 0.158602 Fe  
0.379346 0.093115 0.283326 Fe  
0.874491 0.973067 0.910153 Fe  
0.379170 0.344248 0.033473 Fe  
0.878723 0.218608 0.658675 Fe  
0.380086 0.593761 0.783701 Fe  
0.878499 0.470201 0.408732 Fe  
0.120789 0.280464 0.341382 Fe  
0.621613 0.154795 0.965812 Fe  
0.122915 0.532006 0.090061 Fe  
0.621572 0.406654 0.716503 Fe  
0.123408 0.776216 0.840438 Fe  
0.621512 0.655394 0.466626 Fe  
0.120606 0.030603 0.591620 Fe  
0.621608 0.905262 0.216247 Fe  
0.122344 0.401597 0.219261 Fe  
0.622516 0.276841 0.844587 Fe  
0.622686 0.527065 0.594674 Fe  
0.124536 0.897516 0.719006 Fe  
0.623143 0.776579 0.344430 Fe  
0.121078 0.152944 0.470034 Fe  
0.621758 0.026251 0.094347 Fe  
0.377115 0.723043 0.155344 Fe  
0.882848 0.597524 0.779761 Fe  
0.376791 0.972860 0.905273 Fe  
0.877310 0.849015 0.530993 Fe  
0.376907 0.223494 0.655723 Fe  
0.875831 0.099038 0.280913 Fe  
0.378021 0.472557 0.405381 Fe  
0.877495 0.348293 0.030892 Fe  
0.378160 0.344408 0.533652 Fe  
0.878388 0.219754 0.158935 Fe  
0.379715 0.593655 0.283401 Fe  
0.881141 0.472609 0.909011 Fe

0.375670 0.843034 0.033603 Fe  
0.882804 0.717301 0.658900 Fe  
0.377866 0.093889 0.783822 Fe  
0.877853 0.970758 0.408773 Fe  
0.498844 0.125122 0.375017 N  
-0.000098 0.000113 -0.000497 N  
0.500643 0.374981 0.124953 N  
-0.000872 0.249482 0.750095 N  
0.500365 0.625928 0.875004 N  
-0.000056 0.500510 0.499927 N  
0.500314 0.875240 0.625216 N  
-0.000560 0.749606 0.250060 N  
0.499848 0.625108 0.375264 N  
-0.000222 0.499697 0.000212 N  
0.499534 0.874755 0.124840 N  
0.000915 0.749274 0.750141 N  
0.500434 0.124352 0.874695 N  
0.000561 -0.000486 0.500108 N  
0.500108 0.374769 0.624939 N  
-0.000207 0.249770 0.249891 N  
0.123885 0.034223 0.343964 Ni  
0.853921 0.861192 0.786333 Ni  
0.119157 0.777604 0.339687 Ni  
0.118650 0.648989 0.969969 Ni

**x/16 = 0.0625:**

Fe60 Ni4 N8

1.0

11.341470 0.002219 6.246936

11.339784 5.651339 0.005130

0.001750 5.653436 6.245770

Fe N Ni

60 8 4

direct

0.378173 0.621490 0.876378 Fe

0.622356 0.877796 0.628617 Fe

0.128439 0.371523 0.122406 Fe

0.253618 -0.000482 0.001812 Fe

0.495135 0.251049 0.750245 Fe

0.749346 0.499888 0.499649 Fe

-0.000654 0.750833 0.250937 Fe

0.124948 0.874958 0.626361 Fe

0.373804 0.125610 0.375330 Fe

0.624729 0.375152 0.122369 Fe

0.874312 0.625931 0.874386 Fe

-0.001699 0.252434 0.745951 Fe

0.248299 0.501759 0.499126 Fe

0.500708 0.749083 0.251962 Fe  
0.752784 -0.001996 0.002588 Fe  
0.228070 0.521322 0.978321 Fe  
0.477774 0.772828 0.727216 Fe  
0.728299 0.023250 0.477575 Fe  
0.977664 0.270423 0.227936 Fe  
0.022687 0.728982 0.772256 Fe  
0.271395 0.978239 0.524045 Fe  
0.521562 0.228256 0.272926 Fe  
0.773422 0.476678 0.021241 Fe  
0.352605 0.646275 0.354550 Fe  
0.602308 0.897821 0.101867 Fe  
0.855460 0.147161 0.850634 Fe  
0.100768 0.398986 0.600789 Fe  
0.147752 0.853286 0.147540 Fe  
0.649797 0.349732 0.645897 Fe  
0.896317 0.603833 0.396634 Fe  
0.932905 0.688949 0.067742 Fe  
0.427441 0.192938 0.565757 Fe  
0.681404 0.440365 0.316224 Fe  
0.688134 0.932931 0.312214 Fe  
0.942401 0.180890 0.056525 Fe  
0.186224 0.434223 0.807146 Fe  
0.437547 0.683122 0.563862 Fe  
0.561102 0.316963 0.438804 Fe  
0.812174 0.566320 0.189401 Fe  
0.065285 0.815630 0.939486 Fe  
0.305759 0.072007 0.688023 Fe  
0.317247 0.560839 0.682222 Fe  
0.566658 0.811627 0.433670 Fe  
0.817396 0.060384 0.183675 Fe  
0.066201 0.312617 0.928755 Fe  
0.054336 0.818612 0.445389 Fe  
0.310246 0.061049 0.195625 Fe  
0.558232 0.312500 0.939600 Fe  
0.806412 0.565622 0.691670 Fe  
0.063036 0.307937 0.433948 Fe  
0.314070 0.557570 0.185584 Fe  
0.567470 0.803733 0.939570 Fe  
0.686034 0.442611 0.812634 Fe  
0.935142 0.693323 0.564032 Fe  
0.187345 0.941031 0.314709 Fe  
0.440597 0.188577 0.067322 Fe  
0.443662 0.684707 0.059059 Fe  
0.697415 0.933684 0.810372 Fe  
0.942896 0.184199 0.556392 Fe  
0.192137 0.436082 0.306030 Fe  
-0.000103 -0.000094 0.001046 N

0.248784 0.250791 0.748995 N  
0.500497 0.499731 0.501010 N  
0.748879 0.750933 0.249526 N  
0.126408 0.124075 0.373965 N  
0.376012 0.373592 0.124190 N  
0.624583 0.626216 0.874997 N  
0.873808 0.875554 0.626091 N  
0.874476 0.127077 0.370021 Ni  
0.397394 0.103995 0.895754 Ni  
0.180073 0.939433 0.823512 Ni  
0.812102 0.055556 0.687905 Ni

**x/16 = 0.09375:**

Fe116 Ni12 N16

1.0

11.273283 0.001185 -6.274959  
-11.278102 -0.001682 -6.283813  
0.003843 11.279113 6.279853

Fe N Ni

116 16 12

direct

-0.001189 0.500275 0.750225 Fe  
0.249301 0.248891 0.750027 Fe  
0.499913 -0.000594 0.750969 Fe  
0.749408 0.751024 0.750528 Fe  
0.754394 0.254359 0.249881 Fe  
0.002387 0.000684 0.249242 Fe  
0.247839 0.750440 0.249837 Fe  
0.249859 0.499548 0.001166 Fe  
0.501997 0.251914 -0.000088 Fe  
0.751301 0.000975 0.000419 Fe  
0.750306 0.499987 0.499012 Fe  
0.000726 0.250075 0.499522 Fe  
0.249063 -0.000740 0.497456 Fe  
0.500497 0.750537 0.500179 Fe  
0.250350 0.748127 0.750118 Fe  
0.495078 0.498129 0.748165 Fe  
0.752525 0.252659 0.749529 Fe  
0.747796 0.748984 0.249607 Fe  
0.002756 0.001798 0.749315 Fe  
0.000589 0.500484 0.250636 Fe  
0.251120 0.250905 0.252994 Fe  
0.495961 -0.004594 0.249823 Fe  
0.497759 0.748950 -0.002070 Fe  
0.746647 0.497433 -0.001637 Fe  
0.000682 0.250089 -0.000201 Fe  
0.251257 0.000933 -0.001664 Fe

0.253418 0.500970 0.503237 Fe  
0.499255 0.251218 0.499695 Fe  
0.747875 -0.001626 0.499714 Fe  
0.896501 0.647775 0.751428 Fe  
0.147616 0.397653 0.750025 Fe  
0.396439 0.146438 0.749748 Fe  
0.397091 0.645474 0.249255 Fe  
0.648886 0.898894 0.750386 Fe  
0.645046 0.395618 0.248528 Fe  
0.896852 0.147451 0.250931 Fe  
0.103483 0.852475 0.748338 Fe  
0.601062 0.353670 0.748025 Fe  
0.603594 0.854859 0.250619 Fe  
0.854187 0.103847 0.749621 Fe  
0.852814 0.604065 0.252385 Fe  
0.104827 0.353706 0.250666 Fe  
0.352287 0.102025 0.249580 Fe  
0.896306 0.395914 -0.000630 Fe  
0.146895 0.145917 -0.000051 Fe  
0.396378 0.896709 -0.000630 Fe  
0.646227 0.646205 0.000103 Fe  
0.646992 0.148527 0.501688 Fe  
0.897814 0.894737 0.498439 Fe  
0.146543 0.647528 0.500443 Fe  
0.102078 0.604019 0.000386 Fe  
0.354993 0.354510 0.003283 Fe  
0.603129 0.102963 -0.000251 Fe  
0.601547 0.602460 0.498483 Fe  
0.855041 0.851344 -0.000127 Fe  
0.852935 0.353564 0.499591 Fe  
0.100736 0.099929 0.498982 Fe  
0.353169 0.854063 0.500473 Fe  
0.245371 0.624363 0.878613 Fe  
0.499400 0.378231 0.877142 Fe  
0.497232 0.874909 0.377192 Fe  
0.751344 0.128941 0.877653 Fe  
0.750383 0.627901 0.379035 Fe  
0.003474 0.380798 0.378468 Fe  
0.252017 0.131092 0.380831 Fe  
0.124618 0.001899 0.119609 Fe  
0.370361 0.749361 0.121809 Fe  
0.622742 0.500799 0.121834 Fe  
0.621513 0.002102 0.622424 Fe  
0.872827 0.250848 0.121735 Fe  
0.873059 0.752158 0.624932 Fe  
0.117832 0.496540 0.621088 Fe  
0.367023 0.244100 0.620804 Fe  
0.382679 0.004810 0.381472 Fe

0.629122 0.750732 0.378465 Fe  
0.877415 0.498994 0.377708 Fe  
0.880267 -0.000307 0.878139 Fe  
0.127631 0.247890 0.379834 Fe  
0.128751 0.753203 0.878508 Fe  
0.375166 0.496620 0.878602 Fe  
0.628023 0.248985 0.875674 Fe  
-0.000167 0.622563 0.622704 Fe  
0.246117 0.365968 0.621293 Fe  
0.500358 0.622914 0.121872 Fe  
0.750610 0.872225 0.622443 Fe  
0.751601 0.373743 0.121161 Fe  
0.001593 0.123123 0.122722 Fe  
0.250052 0.873018 0.120521 Fe  
-0.004000 0.625594 0.127516 Fe  
0.248891 0.375818 0.128532 Fe  
0.505891 0.634034 0.630369 Fe  
0.749934 0.877563 0.127347 Fe  
0.749064 0.379910 0.626653 Fe  
-0.000657 0.127689 0.627015 Fe  
0.251936 0.878931 0.628011 Fe  
0.116228 0.747779 0.371545 Fe  
0.375736 0.504319 0.372581 Fe  
0.620773 0.247014 0.369566 Fe  
0.624352 0.752787 0.871285 Fe  
0.870352 -0.000255 0.371459 Fe  
0.870677 0.499042 0.871900 Fe  
0.122659 0.250569 0.871860 Fe  
0.372767 0.000488 0.873176 Fe  
0.382416 0.753327 0.629503 Fe  
0.877693 0.249199 0.626059 Fe  
0.874373 0.746751 0.130766 Fe  
0.129644 0.000005 0.626423 Fe  
0.128486 0.500228 0.128544 Fe  
0.377471 0.246638 0.128392 Fe  
0.628293 0.002733 0.130620 Fe  
0.000808 0.372672 0.871193 Fe  
0.252198 0.123482 0.872280 Fe  
0.503176 0.873833 0.872156 Fe  
0.503824 0.375009 0.374407 Fe  
0.745604 0.619351 0.869871 Fe  
0.249349 0.621167 0.372778 Fe  
0.249054 0.749377 -0.000965 N  
0.498857 0.499706 -0.000459 N  
0.749377 0.249603 -0.000733 N  
0.750452 0.749916 0.501320 N  
-0.000111 -0.000001 0.000140 N  
0.000477 0.499971 0.499937 N

0.250143 0.249384 0.501729 N  
0.500285 -0.000465 0.499282 N  
0.251020 0.500394 0.250775 N  
0.500197 0.250698 0.252152 N  
0.749789 -0.000293 0.248887 N  
0.749094 0.499982 0.749542 N  
-0.002025 0.747141 0.247792 N  
0.000645 0.250801 0.749524 N  
0.250535 -0.000332 0.750145 N  
0.501316 0.750400 0.749823 N  
0.500297 0.499552 0.249182 Ni  
-0.001564 0.748560 0.001972 Ni  
-0.000847 0.748105 0.501940 Ni  
0.146405 0.894988 0.248687 Ni  
0.353345 0.603530 0.749820 Ni  
0.395562 0.398260 0.501112 Ni  
0.000552 0.881490 0.878810 Ni  
0.499816 0.118518 0.619977 Ni  
0.501268 0.130587 0.132570 Ni  
0.630768 0.501846 0.629972 Ni  
0.748868 0.119860 0.368357 Ni  
-0.000260 0.870050 0.367265 Ni

**x/16 = 0.125:**

Fe28 Ni4 N4  
1.0  
0.000927 -5.617738 6.295608  
0.000059 5.623112 6.300657  
-5.626747 -0.002255 -6.298616  
Fe N Ni  
28 4 4  
direct  
0.374969 0.873166 -0.001448 Fe  
0.877376 0.375217 0.003529 Fe  
0.877300 0.876861 0.499117 Fe  
0.129499 0.629703 0.003444 Fe  
0.620345 0.120510 -0.005477 Fe  
0.625586 0.631292 0.502713 Fe  
0.126531 0.121826 0.500403 Fe  
0.599675 0.103107 0.498370 Fe  
0.102972 0.599182 0.498238 Fe  
0.894919 0.397294 0.501052 Fe  
0.357197 0.353654 0.002655 Fe  
0.852655 0.854051 -0.000769 Fe  
0.148153 0.149145 0.003029 Fe  
0.646578 0.645153 -0.002755 Fe  
0.505982 0.262602 0.763113 Fe

-0.001186 0.756292 0.752192 Fe  
0.252083 0.498276 0.754534 Fe  
0.760586 0.004153 0.756982 Fe  
0.244196 0.000584 0.240407 Fe  
0.506018 0.745390 0.245161 Fe  
-0.005125 0.243037 0.242443 Fe  
0.250140 0.506876 0.257982 Fe  
0.751129 0.005591 0.254601 Fe  
0.006642 0.746663 0.254743 Fe  
0.507446 0.254172 0.263355 Fe  
0.492750 0.745181 0.740213 Fe  
0.993836 0.252697 0.746865 Fe  
0.248210 0.989288 0.742837 Fe  
-0.001147 -0.000152 -0.001459 N  
0.499867 0.502243 0.000973 N  
0.750697 0.249060 0.501814 N  
0.250711 0.748207 0.500572 N  
0.366218 0.370710 0.496291 Ni  
0.395444 0.898800 0.501552 Ni  
0.739566 0.499717 0.240310 Ni  
0.752182 0.490451 0.742419 Ni

**x/16 = 0.15625:**

Fe108 Ni20 N16

1.0

11.215897 0.004234 -6.311403  
-0.007371 -11.247152 -6.317202  
-5.606056 5.616947 -6.311828

Fe N Ni

108 16 20

direct

0.252733 0.000252 0.504819 Fe  
0.753490 0.499599 0.503117 Fe  
0.001593 0.749602 -0.001337 Fe  
0.375544 0.626022 0.751444 Fe  
0.125722 0.375993 0.250921 Fe  
0.500526 0.249187 -0.002250 Fe  
0.872527 0.122078 0.743654 Fe  
0.497113 0.753984 0.502216 Fe  
0.876470 0.628576 0.252670 Fe  
0.001508 0.251513 0.508260 Fe  
0.247482 0.499147 -0.005965 Fe  
0.378408 0.124572 0.254314 Fe  
0.749576 0.000807 -0.000987 Fe  
0.125473 0.872164 0.743695 Fe  
0.373907 0.124914 0.752986 Fe  
0.750662 -0.000791 0.498873 Fe



0.871548 0.623893 0.748781 Fe  
0.124711 0.879258 0.244441 Fe  
0.500193 0.747308 -0.000725 Fe  
0.625393 0.377333 0.247809 Fe  
0.001140 0.251554 0.007328 Fe  
0.623334 0.871497 0.749726 Fe  
-0.000899 0.748832 0.496860 Fe  
0.125130 0.374868 0.751640 Fe  
0.748271 0.503194 0.002735 Fe  
0.498905 0.250437 0.497024 Fe  
0.874986 0.123021 0.242303 Fe  
0.073570 0.072190 0.645978 Fe  
0.573106 0.572655 0.649454 Fe  
0.824201 0.824596 0.145753 Fe  
0.198593 0.698340 0.894070 Fe  
0.950721 0.445473 0.397053 Fe  
0.322741 0.323563 0.145669 Fe  
0.697238 0.198665 0.893780 Fe  
0.176458 0.175806 0.856759 Fe  
0.550628 0.050968 0.603038 Fe  
0.927542 0.928459 0.351549 Fe  
0.301262 0.801231 0.101981 Fe  
0.053591 0.551345 0.602422 Fe  
0.426333 0.428100 0.353193 Fe  
0.802539 0.302434 0.104591 Fe  
0.200445 0.697104 0.397779 Fe  
0.697778 0.198803 0.394151 Fe  
0.946088 0.447598 0.898862 Fe  
0.323060 0.324245 0.645439 Fe  
0.447292 0.948027 0.902233 Fe  
0.823371 0.822019 0.645521 Fe  
0.675169 0.677914 0.351744 Fe  
0.798827 0.301679 0.606371 Fe  
0.053731 0.553892 0.101682 Fe  
0.427096 0.425167 0.851063 Fe  
0.177735 0.176337 0.354151 Fe  
0.553032 0.050168 0.104747 Fe  
0.926949 0.926682 0.848768 Fe  
0.436227 0.938164 0.637795 Fe  
0.558798 0.559030 0.877165 Fe  
0.812666 0.811875 0.378344 Fe  
0.936835 0.436210 0.631035 Fe  
0.310520 0.310762 0.376052 Fe  
0.686378 0.186723 0.125312 Fe  
0.120428 0.879881 -0.006646 Fe  
0.492812 0.753137 0.748756 Fe  
0.621742 0.377407 -0.005935 Fe  
0.872403 0.628456 0.500819 Fe

0.246663 0.503488 0.242735 Fe  
0.996230 0.252274 0.757789 Fe  
0.372703 0.129966 0.504118 Fe  
0.748065 0.003172 0.247045 Fe  
0.376043 0.619627 -0.001477 Fe  
0.751328 0.493088 0.751961 Fe  
0.877588 0.120730 -0.009089 Fe  
0.129003 0.372372 0.503068 Fe  
0.502353 0.247817 0.247560 Fe  
0.251965 0.998060 0.757524 Fe  
0.630112 0.872896 0.504548 Fe  
0.005522 0.747470 0.246628 Fe  
0.188889 0.188642 0.624511 Fe  
0.566648 0.065706 0.375267 Fe  
0.685600 0.686553 0.616539 Fe  
0.938606 0.938090 0.116477 Fe  
0.314736 0.815447 0.876256 Fe  
0.064066 0.562962 0.371124 Fe  
0.437244 0.437158 0.115782 Fe  
0.564182 0.563377 0.384921 Fe  
0.683732 0.183222 0.621850 Fe  
0.311002 0.311154 0.878308 Fe  
0.061539 0.064115 0.381052 Fe  
0.436435 0.933822 0.129176 Fe  
0.247229 0.504154 0.746946 Fe  
0.746126 0.001157 0.747751 Fe  
0.372884 0.127971 0.002808 Fe  
0.496671 0.754986 0.251135 Fe  
0.872537 0.631425 0.002365 Fe  
0.501724 0.245107 0.747342 Fe  
0.003274 0.746760 0.748066 Fe  
0.256326 0.998666 0.256040 Fe  
0.630279 0.871325 0.000163 Fe  
0.375733 0.622207 0.500839 Fe  
0.756869 0.498680 0.254015 Fe  
0.126231 0.371999 0.001820 Fe  
0.309501 0.813372 0.365777 Fe  
0.691100 0.690844 0.125380 Fe  
0.815542 0.311505 0.373580 Fe  
0.060566 0.562623 0.868101 Fe  
0.442164 0.438519 0.622503 Fe  
0.190838 0.190896 0.127521 Fe  
0.563352 0.061829 0.870955 Fe  
0.939843 0.937962 0.616352 Fe  
0.372845 0.876246 0.752933 N  
0.749549 0.749130 0.498864 N  
0.874929 0.373621 0.751526 N  
0.126385 0.625989 0.250498 N

0.500275 0.499435 -0.000988 N  
0.249773 0.249603 0.500823 N  
0.625212 0.125556 0.248362 N  
-0.001694 0.000371 -0.001986 N  
0.499645 0.501572 0.499510 N  
0.875356 0.374421 0.250971 N  
0.000917 0.001134 0.498002 N  
0.249577 0.249777 0.000648 N  
0.624388 0.123957 0.749339 N  
0.374461 0.874590 0.250096 N  
0.749444 0.749599 0.003579 N  
0.124473 0.625212 0.749468 N  
0.625212 0.878384 0.255586 Ni  
0.624255 0.371284 0.746111 Ni  
0.251136 0.497109 0.494523 Ni  
0.381440 0.623483 0.253772 Ni  
0.251470 0.001589 0.007814 Ni  
0.449047 0.947531 0.399291 Ni  
0.676473 0.676478 0.855073 Ni  
0.571637 0.572879 0.148310 Ni  
0.073704 0.072296 0.145412 Ni  
0.300042 0.804428 0.603002 Ni  
0.058898 0.061810 0.879771 Ni  
0.187575 0.685453 0.130676 Ni  
0.816135 0.312255 0.871341 Ni  
0.186348 0.682906 0.628120 Ni  
0.934158 0.440242 0.134500 Ni  
0.809556 0.809652 0.879390 Ni  
0.620896 0.380838 0.495273 Ni  
0.995049 0.253344 0.255735 Ni  
0.119812 0.879195 0.491517 Ni  
0.879236 0.121520 0.495148 Ni

**x/16 = 0.1875:**

Fe52 Ni12 N8  
1.0  
-5.634188 -5.569030 6.311099  
5.639338 5.572387 6.318733  
-5.635089 5.564797 -6.315626  
Fe N Ni  
52 8 12  
direct  
0.632818 0.885495 0.257945 Fe  
0.128835 0.880201 0.749107 Fe  
0.124505 0.375063 0.250771 Fe  
0.876025 0.126482 0.745830 Fe  
0.868256 0.619132 0.252127 Fe

0.376552 0.626092 0.750448 Fe  
0.369726 0.622211 0.250149 Fe  
0.873827 0.626461 0.756359 Fe  
0.874303 0.121728 0.245469 Fe  
0.373215 0.123409 0.751099 Fe  
0.126556 0.875776 0.241635 Fe  
0.625024 0.870548 0.752156 Fe  
0.125517 0.380212 0.755873 Fe  
0.853801 0.852630 0.497366 Fe  
0.353947 0.855519 0.003957 Fe  
0.353577 0.350517 0.498511 Fe  
0.849248 0.353696 -0.001096 Fe  
0.644095 0.642732 0.494605 Fe  
0.146686 0.143752 0.496608 Fe  
0.646866 0.147640 0.002227 Fe  
0.854640 0.354528 0.502040 Fe  
0.354641 0.357764 0.002204 Fe  
0.354223 0.851474 0.502184 Fe  
0.147444 0.146138 -0.001821 Fe  
0.145422 0.647196 0.503148 Fe  
0.646276 0.645708 -0.001739 Fe  
0.880956 0.877717 0.753165 Fe  
0.380602 0.876103 0.255973 Fe  
0.373172 0.377561 0.756284 Fe  
0.878226 0.378959 0.257357 Fe  
0.880688 0.123676 -0.003794 Fe  
0.377819 0.116254 0.504156 Fe  
0.618264 0.372845 -0.006931 Fe  
0.124274 0.379201 0.503238 Fe  
0.124006 0.880415 -0.006924 Fe  
0.618767 0.875169 0.502370 Fe  
0.620633 0.626945 0.243044 Fe  
0.122876 0.121712 0.241179 Fe  
0.876421 0.380535 0.760365 Fe  
0.375825 0.374308 0.253481 Fe  
0.380068 0.880559 0.757660 Fe  
0.878315 0.871839 0.255358 Fe  
0.377074 0.620651 0.500522 Fe  
0.381132 0.127489 0.003583 Fe  
0.885336 0.129937 0.501412 Fe  
0.617570 0.875204 0.001742 Fe  
0.116377 0.372900 -0.000316 Fe  
0.626484 0.380371 0.497044 Fe  
0.626711 0.129665 0.247678 Fe  
0.123327 0.122748 0.741968 Fe  
0.114496 0.621875 0.244104 Fe  
0.618073 0.616619 0.742058 Fe  
0.498038 -0.005474 0.496723 N

-0.000202 -0.001344 -0.003108 N  
0.000735 0.499205 0.502224 N  
0.500159 0.500896 -0.001130 N  
0.499399 0.497909 0.498731 N  
0.000163 0.498323 0.002038 N  
-0.001056 0.000712 0.497990 N  
0.500812 0.001401 0.003397 N  
0.621188 0.372385 0.743381 Ni  
0.376288 0.122088 0.254475 Ni  
0.628537 0.383162 0.247705 Ni  
0.145018 0.644073 -0.001719 Ni  
0.852346 0.853899 -0.002182 Ni  
0.645181 0.145116 0.499818 Ni  
0.386668 0.628221 0.009213 Ni  
0.883744 0.623455 0.511606 Ni  
0.119741 0.626110 0.742442 Ni  
0.620295 0.116161 0.740086 Ni  
0.881300 0.621983 0.004591 Ni  
0.118125 0.878361 0.490784 Ni