Supplementary information for The promoter role of sulfur in the growth efficiency of carbon nanotubes

Balázs Orbán[1]. Tibor Höltzl[1.2.3]

1. Budapest University of Technology and Economics. Szent Gellért tér 4. H1111. Budapest. Hungary
2. MTA-BME Computation Driven Research Group. Szent Gellért tér 4. H1111. Budapest. Hungary
3. Furukawa Electric Institute of Technology. Késmárk utca 28/A. H1158. Budapest. Hungary

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1. Computation method for graphene – metal system

Although the adsorption of graphene to many 3d, 4d and 5d transition metals have been calculated before, iron – graphene interaction is rare in the literature. Thus, we chose nickel as a reference metal system to verify the selected C09-vdW-DF functional and find the appropriate calculation parameters. There are several previous studies on the adsorption of graphene on Ni fcc(111) surface as nickel is commonly used catalyst for the CVD growth of graphene.

For the convergence of plane-wave cutoff energy (PW cutoff) and number of Monkhorst-Pack k-points, a (2x2) orthogonal Ni slab consisting of 3 atomic layers was used with a graphene layer on top of it. First, we converged PW cutoff with 8x8x1 k-points and the calculated total energies (E_{total}) are listed in **Table S1** where E_{diff} represents the difference in total energies of the given row and the previous one. Then we performed the k-point

convergence with the chosen cutoff energy of 500 eV which is shown in **Table S2**. Based on the results we selected 10x10x1 k-points because further increase of the number of k-points shows negligible difference in the total energy.

Table S1. Total energy of graphene on Ni(2x2x3) slab with fcc(111) arrangement as a function of plane-wave cutoff energy.

PW cutoff [eV]	**E_{total} [eV]**	**E_{diff} [eV]**
200	-999.1969	-
250	-1022.5878	23.391
300	-1031.3663	8.778
350	-1035.2320	3.866
400	-1036.9673	1.735
450	-1037.7105	0.743
500	**-1038.0042**	**0.294**
550	-1038.0863	0.082
600	-1038.1079	0.022
650	-1038.1219	0.014
700	-1038.1392	0.017

Table S2. Total energy of graphene on Ni(2x2x3) slab with fcc(111) arrangement as a function of k-points in the two periodic directions.

K-points	**E_{total} [eV]**	**E_{diff} [eV]**
2x2x1	183.7594	-
4x4x1	183.8548	-0.09536
6x6x1	183.9195	-0.06472
8x8x1	183.9021	0.01746
10x10x1	**183.9049**	**-0.00281**
12x12x1	183.9044	0.00044
14x14x1	183.9040	0.00041
16x16x1	183.9042	-0.00017
18x18x1	183.9041	0.00006

Then the unit cell of Ni and Fe slabs with fcc structure was optimized. The parameters of the (2x2) orthogonal cell considering six atomic layers are listed in **Table S3**. Spin-polarization has a negligible effect on the size of the cell, the difference is less than 0.01 Å in the lattice constant for both metals.

Table S3. Optimized cell parameters of Ni and Fe slab with fcc structure of six atomic layers without spin polarization.

	Ni			**Fe**		
	x	y	z	x	y	z
A	4.972559	-0.000146	0.000314	4.867366	0.0	0.0
B	-0.000126	4.304575	-0.001030	0.0	4.215396	6.5e-05
C	0.000773	-0.002912	12.216619	0.0	0.000187	11.949321

The vacuum region above the surface of the metal slab was also optimized to avoid the interaction between the replicas of the system (**Figure S1**). We found that a vaccum of 15 Å is appropriate even if a bigger graphene – metal surface distance is considered in the potential energy surface calculation.

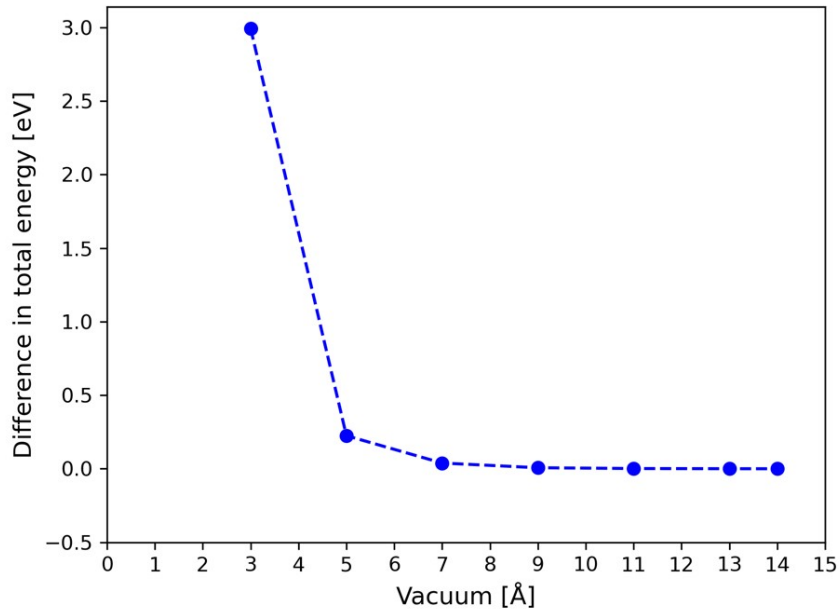

Figure S1. Difference in total energy of Ni(2x2x3) with fcc(111) arrangement as a function of vacuum region above it.

2. Effect of magnetism on the binding energy of graphene

As a reference of our computation method we calculated the binding energy of graphene to Ni fcc(111) surface as a function of distance between graphene and Ni surface. The bottom three atomic layers of Ni slab was fixed in the optimization to save computational time (instead of the calculations shown in the main text in which only the bottom layer was fixed). We considered the three most commonly studied adsorption site (top-fcc, top-hcp and fcc-hcp) of graphene in spin-unpolarized and spin-polarized case, too. Our results are shown in **Figure S2**. In case of the same graphene configuration spin polarization barely affects the binding energy comparing to spin-unpolarized calculation. the difference is 20 meV around the equilibrium distance in tf and th sites.

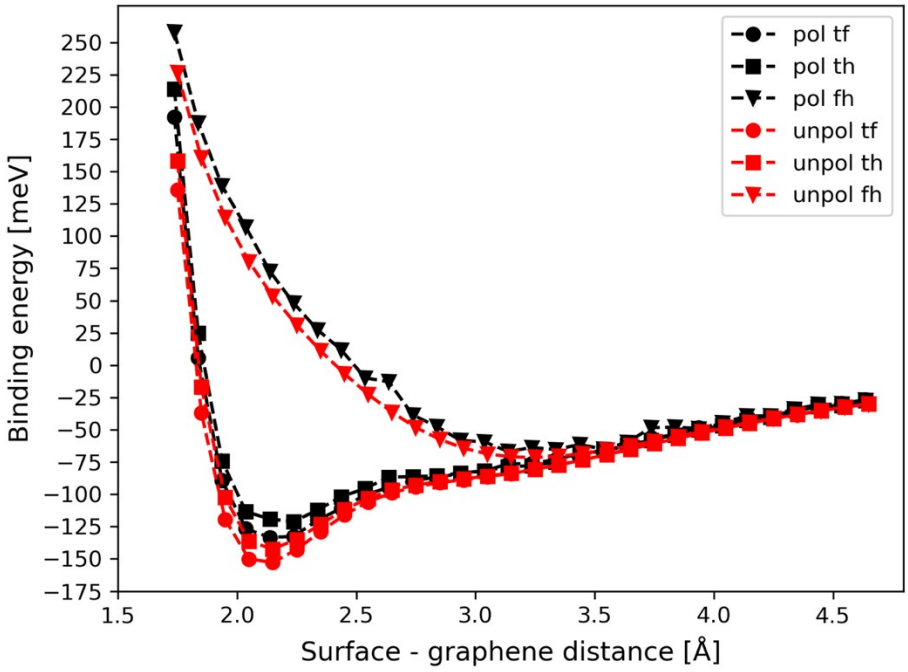

Figure S2. Binding energy of graphene to Ni fcc(111) surface as a function of graphene – metal surface distance.

The same calculation was performed for Fe fcc(111) surface and the results are summarized in **Figure S3**. The difference between spin-polarized and spin-unpolarized calculations is negligible for Fe, too. Equilibrium distances are the same while deviation in binding energies are less than 15 meV.

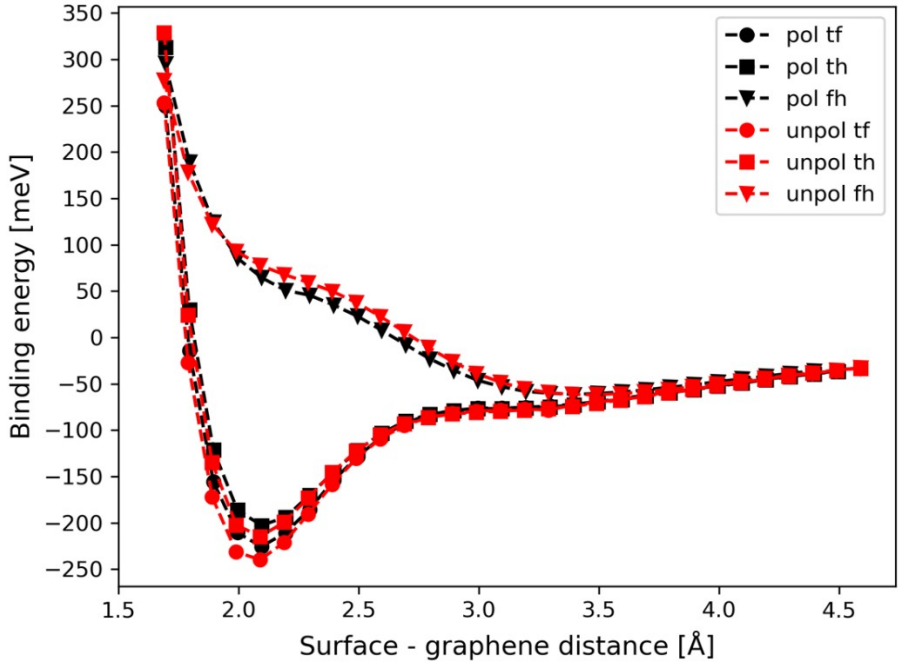

Figure S3. Binding energy of graphene to Fe fcc(111) surface as a function of graphene – metal surface distance.

The effect of magnetism was also investigated in NP-nanocap and NP-CNT systems. The calculated binding energies considering both spin-polarized and spin-unpolarized case are shown in **Table S4**. There is a noticeable difference in binding energy between spin-polarized and spin-unpolarized calculation of the same system, varying in the range of 0.2 – 0.7 eV. However, both cases show the same tendency in the change of binding energy considering the different sulfur substitution and content.

Table S4. Calculated binding energies of Fe_{13} with CNT(5,0) and Fe_{55} with CNT(10,0).

Nanoparticle		**Binding energy (NP-cap) [eV]**		**Binding energy (NP-CNT) [eV]**	
		Spin-unpol.	**Spin-pol.**	**Spin-unpol.**	**Spin-pol.**
Fe_{13}		-3.64	-3.17	-3.11	-2.74
Fe_{12}		-3.27	-2.80	-2.60	-2.22
$Fe_{12}S$	**Top**	-2.67	-2.05	-1.93	-1.54
	Edge	-3.55	-2.84	-2.93	-2.39
	Bottom	-3.72	-3.00	-3.24	-2.46
Fe_{55}		-3.70	-3.17	-3.81	-3.21
$Fe_{54}S$		-3.72	-3.16	-3.81	-3.21
$Fe_{52}S_3$		-2.86	-2.45	-3.01	-2.58
$Fe_{49}S_6$		-2.01	-1.80	-2.13	-1.89

3. The adsorption of graphene on partially sulfur-covered Fe fcc(111) surfaces

To investigate the effect of partial sulfur coverage on the graphene adsorption, along with the results using the (2x2) Fe fcc(111) orthogonal cell in the main text, we also computed the (4x4) orthogonal cell with three atomic layers. The optimized structure is shown in **Figure S4**. The structure of the surface bound graphene is slightly corrugated, which is energetically favoured, as it somewhat reduces the metal-carbon distances at sulfur-free part of the iron surface (**Figure 2**). However, corrugation is small (only ~ 0.2Å), thus is expected to play a minor role in the FCCVD process.

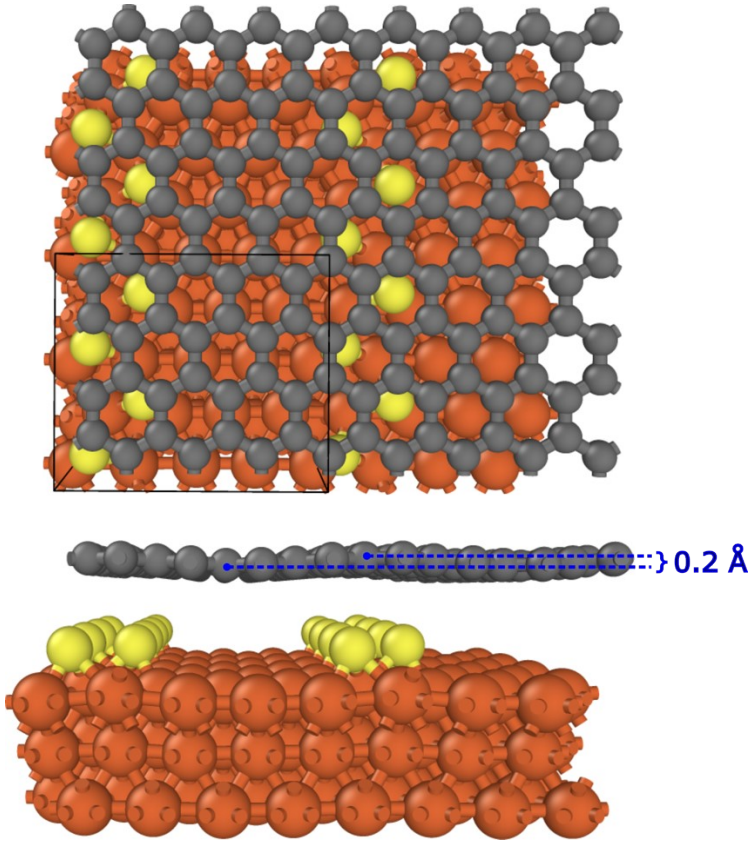

Figure S4. Optimized structure of graphene adsorbed on partially sulfur-covered iron surface. Black rectangle represents the applied cell in the computations.

4. Geometry optimization of Fe_{55} based systems

The geometry optimization was performed using linear combination of atomic orbitals (LCAO) method with triple-zeta basis set (TZP) due to the much lower computational cost and the optimization criterion was set to 0.02 eV/Å on each atom. For the final energies, single point computations were performed on the optimized geometries using the plane wave basis set and the method described above. Our preliminary calculations showed that the difference between the two optimization methods is relatively small, even the biggest deviation in binding energy of CNT to M_{55} is less than 10^{-3} eV.

5. Non-covalent interaction (NCI) calculation of Fe_{55}, $Fe_{54}S$ and $Fe_{49}S_6$ with nanocap

The non-covalent interaction between CNT(10,0) nanocap and Fe_{55}, $Fe_{54}S$ and $Fe_{49}S_6$ was calculated. The reduced gradient (s) as a function of the second eigenvalue of the Hessian (λ_2) is presented in **Figure S5**.

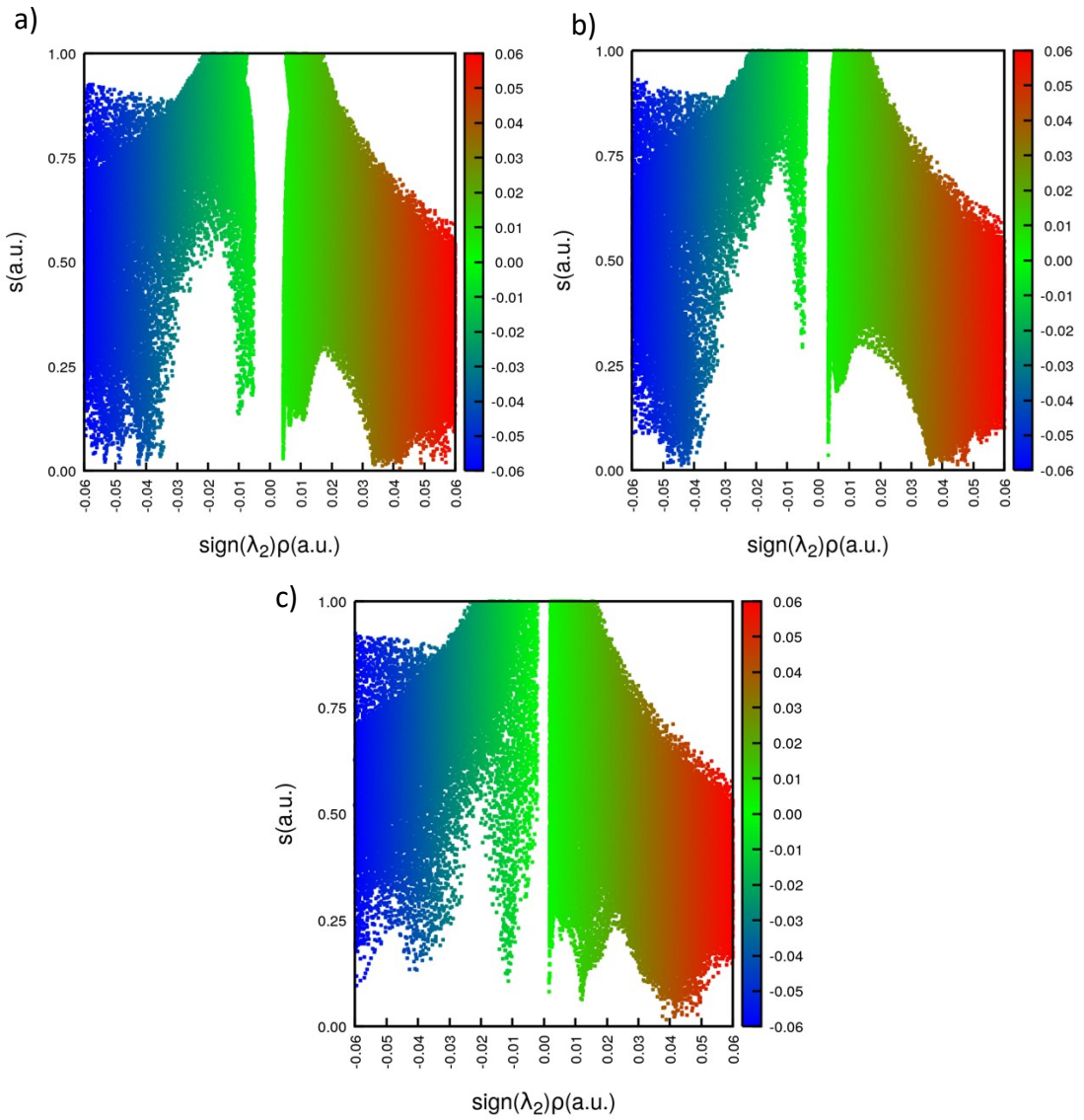

Figure S5. NCI plot of nanocap binding to a) Fe_{55}, b) $Fe_{54}S$ and c) $Fe_{49}S_6$.

In comparison of Fe_{55} and $Fe_{54}S$ there is only a small difference in the region of weak interaction ($-0.02 < \lambda_2 < 0.02$) which shows the reduction in the interaction due to the substitution of top atom (under nanocap) in the NP. However, in case of $Fe_{49}S_6$ there is a significant change in the $-0.06 < \lambda_2 < -0.03$ region which belongs to the strong and attractive interactions. For $Fe_{49}S_6$ the attractive interaction reduces, indicating a weaker binding of the nanocap to the nanoparticle.

6. Molecular Dynamics simulation of $Fe_{12}S$+nanocap(5,0) and $Fe_{52}S_3$+nanocap(10,0)

We performed Density Functional Theory based molecular dynamics (MD) simulation using the revised PBE functional, D3 dispersion correction and the double-zeta basis set on the $Fe_{12}S$ with nanocap (5,0) (Top configuration) and $Fe_{52}S_3$ with nanocap (10,0). The optimized structures reported in the main text were used as initial structures for the simulation. The simulation timestep was set to 0.5 fs and temperature was kept at 1000 Kelvin. The results are shown in **Figure S6**. We performed geometry optimization from the final step of the molecular dynamics simulation to calculate binding energy (E_b) using the original method, as it is described in the main text. (**Figure S6c)**.

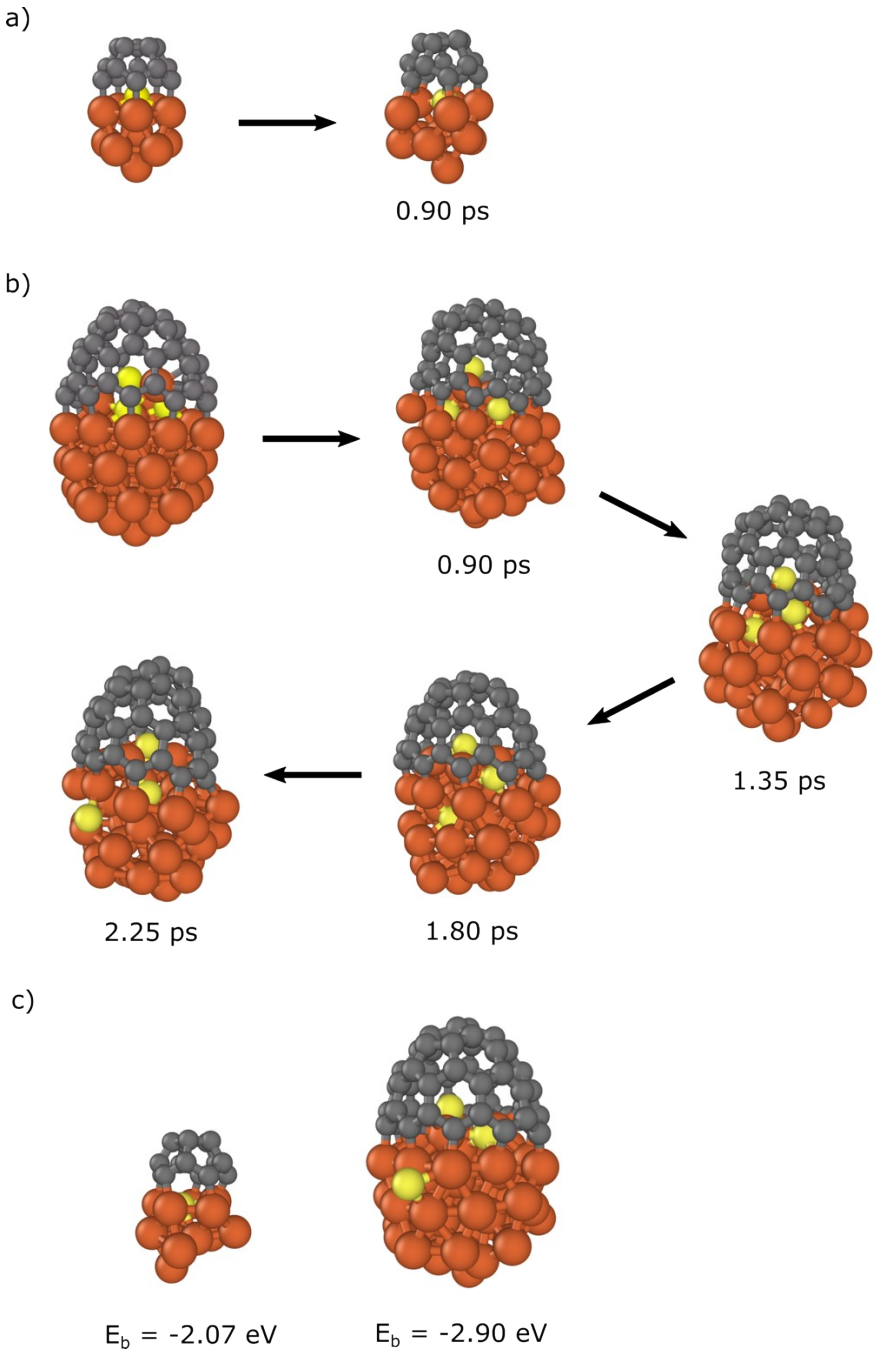

Figure S6. Snapshots along the molecular dynamics trajectories of a) $Fe_{12}S$+nanocap (5,0) and b) $Fe_{52}S_3$+nanocap(10,0) at 1000 Kelvin with simulation timestep of 0.5 fs and c) their optimized structures carried out from the final step.

For $Fe_{12}S$+nanocap (5,0) (**Figure S6a**), after 0.90 ps molecular dynamics simulation a similar geometrical structure is observed to the initial configuration (with a sulfur atom under the cap). The binding energy is -2.07 eV with a very small difference compared to that of the initial structure (-2.05 eV). However, in the case of $Fe_{52}S_3$+nanocap (10,0) (**Figure S6b**) a sulfur atom migrates from the region under the cap. This can occur due to the molten surface layer of the NP at the temperature used in the simulation. Thus, the binding of nanocap becomes stronger (E_b = -2.90 eV) compared to the initial structure where three sulfur atoms reside under the cap (E_b = -2.45 eV). The final optimization reproduced the icosahedral configuration of $Fe_{52}S_3$ that supports the choice of icosahedral structure as model system for iron nanoparticles.

This suggests that sulfur can easily migrate along the molten surface layer of the NP during cap growth, and thus the sulfur content under the cap depends on the sulfur coverage of the whole nanoparticle.

7. Atomic positions of the optimized structures

Graphene in Ni cell

C 2.52342437 3.96993809 6.20682610
C 1.27772498 1.81155441 6.20693502
C 2.52343621 1.09201765 6.20652703
C 1.27772482 3.25040866 6.20703606
C 5.01487645 3.96996864 6.20702690
C 3.76919205 1.81151421 6.20661896
C 5.01488795 1.09197099 6.20672758
C 3.76919188 3.25043375 6.20671917

Graphene in Fe cell

C 2.53787400 3.93608500 6.20669900
C 1.32102900 1.82845200 6.20713400
C 2.53787400 1.12587200 6.20668000
C 1.32102900 3.23350600 6.20713300
C 4.97156500 3.93609000 6.20711300
C 3.75472200 1.82844800 6.20670400
C 4.97156600 1.12586800 6.20709600
C 3.75472300 3.23351000 6.20601000

Ni(2x2x6) slab

Ni 1.24570400 0.71931500 -0.00014400
Ni 3.73707300 0.71930700 -0.00024400
Ni -0.00001000 2.87774300 0.00019900
Ni 2.49138100 2.87773400 0.00010100
Ni -0.00008600 1.43903500 2.03402600
Ni 2.49130500 1.43902600 2.03392600
Ni 1.24561500 3.59745300 2.03427300
Ni 3.73698200 3.59744400 2.03417400
Ni -0.00016200 0.00032800 4.06791300
Ni 2.49122900 0.00032000 4.06781800
Ni 1.24553800 2.15874600 4.06816300
Ni 3.73690600 2.15873800 4.06806300
Ni 1.24545189 0.72007155 6.10608510
Ni 3.73684450 0.72006368 6.10598572
Ni -0.00025043 2.87849840 6.10642787
Ni 2.49114115 2.87849150 6.10633328
Ni -0.00031859 1.43990363 8.14425972
Ni 2.49107294 1.43989510 8.14416092
Ni 1.24537010 3.59832213 8.14450567
Ni 3.73676176 3.59831420 8.14440639
Ni -0.00037950 0.00116032 10.16059484
Ni 2.49101213 0.00115257 10.16049717
Ni 1.24530975 2.15957942 10.16084182
Ni 3.73670048 2.15957143 10.16074270

Fe(2x2x6) slab

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe -0.00000022 1.40174107 2.00378749
Fe 2.43368278 1.40174113 2.00378730
Fe 1.21684202 3.51984264 2.03364412
Fe 3.65052358 3.51984264 2.03364412
Fe -0.00000021 0.04068683 4.01346648
Fe 2.43368279 0.04068698 4.01346627
Fe 1.21684191 2.14097882 4.03438995
Fe 3.65052365 2.14097882 4.03438994
Fe 1.21684191 0.78598273 6.03643638
Fe 3.65052366 0.78598273 6.03643638
Fe -0.00000022 2.88859777 6.06585627
Fe 2.43368278 2.88859775 6.06585639
Fe -0.00000022 1.52745079 8.06373815
Fe 2.43368278 1.52745081 8.06373813
Fe 1.21684202 3.63403383 8.05639107
Fe 3.65052354 3.63403383 8.05639106
Fe -0.00000022 0.13759085 10.12805265
Fe 2.43368278 0.13759091 10.12805248
Fe 1.21684205 2.23490307 10.03974917
Fe 3.65052351 2.23490307 10.03974917

Fe(2x2x6)S_1 slab

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe -0.00024480 1.40087159 1.99771985
Fe 2.43389850 1.40087168 1.99771975
Fe 1.21682532 3.51789383 2.03075730
Fe 3.65050681 3.51978081 2.02806356
Fe -0.00006294 0.03169708 4.01464680
Fe 2.43370241 0.03169716 4.01464663
Fe 1.21682040 2.13227768 4.02602057
Fe 3.65050194 2.13344449 4.02657613
Fe 1.21681445 0.78179607 6.05091649
Fe 3.65049574 0.78342585 6.04286171
Fe 0.00197688 2.88201167 6.03206318
Fe 2.43165021 2.88201163 6.03206299
Fe 0.00076618 1.53046724 8.08302880
Fe 2.43285338 1.53046712 8.08302889
Fe 1.21681060 3.64065286 8.06416521
Fe 3.65049203 3.62644693 8.03034108
Fe -0.00955099 0.15411644 10.03596831
Fe 2.44316728 0.15411648 10.03596882
Fe 1.21680970 2.27938569 10.09341381
Fe 3.65049031 2.29805897 10.05314352
S 1.21680731 0.81687680 11.72664660

Fe(2x2x6)S_2 slab

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe -0.00053167 1.40211933 2.00322804
Fe 2.43292104 1.40214324 2.00177460
Fe 1.21672689 3.51852154 2.03692985
Fe 3.65179895 3.52042178 2.03668920
Fe 0.00288404 0.03902946 4.01935107
Fe 2.43310471 0.03432953 4.02001537
Fe 1.21664236 2.13708606 4.03669942
Fe 3.64798484 2.14184608 4.03639022
Fe 1.22579565 0.77732249 6.05097988
Fe 3.65079330 0.79211615 6.04708112
Fe 0.00015923 2.89710563 6.04832685
Fe 2.42517254 2.88257022 6.05148850
Fe 0.01650637 1.51711435 8.03165974
Fe 2.42657483 1.53073162 8.11161335
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Fe 3.63576414 3.62469376 8.03429568
Fe -0.05715849 0.16680188 9.97269166
Fe 2.36280548 0.18755510 10.21814374
Fe 1.28831896 2.29494560 10.21944262
Fe 3.70608736 2.27296322 9.96897157
S 0.81925828 0.85835977 11.76179021
S 2.83616854 2.96855075 11.75940069

Fe(2x2x6)S_3 slab

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00075991 1.39804683 1.99997302
Fe 2.43443949 1.39862775 1.99730718
Fe 1.21769054 3.51670299 2.03806784
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Fe 0.00110123 0.03714629 4.01657251
Fe 2.43478439 0.03503782 4.02142162
Fe 1.21789636 2.13592662 4.02804367
Fe 3.65166812 2.13592830 4.02804503
Fe 1.22148467 0.78048818 6.05267187
Fe 3.64866819 0.78048737 6.05267696
Fe 0.00139436 2.88055937 6.04064740
Fe 2.43507992 2.87847713 6.03881513
Fe 0.00154816 1.51251425 8.06509108
Fe 2.43523186 1.52556199 8.10518370
Fe 1.21689606 3.61096164 8.02539280
Fe 3.65355059 3.61096756 8.02539863
Fe 0.00165247 0.07509821 10.00666738
Fe 2.43534194 0.10051838 10.07921057
Fe 1.19315372 2.23095260 10.11903108

Fe 3.67751520 2.23095094 10.11902295
S 1.09887714 0.81117495 11.77676237
S 2.43534946 2.93444403 11.79328533
S 3.77183097 0.81118998 11.77676411

Fe(2x2x6)S_4 slab

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00059561 1.41077709 2.04213982
Fe 2.43427856 1.41077691 2.04213987
Fe 1.21735419 3.50843785 2.00369065
Fe 3.65103523 3.50843788 2.00369060
Fe 0.00069983 0.03234678 4.03966206
Fe 2.43438282 0.03234658 4.03966204
Fe 1.21754972 2.14562863 4.02471258
Fe 3.65123091 2.14562879 4.02471259
Fe 1.21766931 0.78338487 6.05761431
Fe 3.65135020 0.78338430 6.05761419
Fe 0.00082965 2.89442572 6.05706510
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Fe 1.21769046 3.62884184 8.06058505
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Fe 0.00081669 0.14130415 10.11620350
Fe 2.43450287 0.14130488 10.11620386
Fe 1.21765927 2.24945972 10.11771815
Fe 3.65134418 2.24945940 10.11771900
S 1.21766406 0.83687369 11.84829062
S 2.43450210 2.94493603 11.85001301
S 3.65134104 0.83687313 11.84830096
S 0.00081994 2.94493518 11.85002256

Graphene on Ni(2x2x6)

Ni 1.24570400 0.71931500 -0.00014400
Ni 3.73707300 0.71930700 -0.00024400
Ni -0.00001000 2.87774300 0.00019900
Ni 2.49138100 2.87773400 0.00010100
Ni -0.00008600 1.43903500 2.03402600
Ni 2.49130500 1.43902600 2.03392600
Ni 1.24561500 3.59745300 2.03427300
Ni 3.73698200 3.59744400 2.03417400
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Ni 1.24546200 0.72015600 6.10196400
Ni 3.73682900 0.72014800 6.10186400
Ni -0.00025200 2.87858300 6.10230700
Ni 2.49113800 2.87857600 6.10220900
Ni -0.00032900 1.43987500 8.13612300

Ni 2.49106200 1.43986700 8.13602400
Ni 1.24536900 3.59829300 8.13637000
Ni 3.73674100 3.59828500 8.13627000
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Ni 2.49098600 0.00115900 10.16980300
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Ni 3.73666400 2.15957700 10.17005000
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C 1.27768300 2.15048000 12.307058
C 5.01491400 2.86990100 12.307052
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C 3.76923300 2.15052800 12.306723

Graphene on Fe(2x2x6)

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00030961 1.40070576 1.99518287
Fe 2.43399262 1.40070581 1.99518270
Fe 1.21720540 3.51898881 2.02380341
Fe 3.65088678 3.51898881 2.02380339
Fe 0.00048725 0.03110868 4.00304969
Fe 2.43417030 0.03110867 4.00304963
Fe 1.21733454 2.13358223 4.02758075
Fe 3.65101596 2.13358222 4.02758074
Fe 1.21749245 0.76399854 6.01972550
Fe 3.65117364 0.76399849 6.01972546
Fe 0.00063926 2.86414210 6.03124390
Fe 2.43432232 2.86414198 6.03124396
Fe 0.00080614 1.48714012 8.04798420
Fe 2.43448932 1.48714021 8.04798454
Fe 1.21766443 3.58082088 8.07361060
Fe 3.65134567 3.58082080 8.07361069
Fe 0.00088177 0.06457475 10.01564673
Fe 2.43456476 0.06457507 10.01564837
Fe 1.21772303 2.16872696 10.01688729
Fe 3.65140533 2.16872689 10.01688778
C 2.43474380 2.86154034 12.05819628
C 1.21790550 0.75363345 12.05208085
C 2.43474937 0.05124718 12.10481828
C 1.21791064 2.15930245 12.10712107
C 4.86842654 2.86153885 12.05819445
C 3.65158179 0.75363352 12.05207983
C 4.86843218 0.05124891 12.10481460
C 3.65158760 2.15930241 12.10712125

Graphene on Fe(2x2x6)S_1

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693

Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00037462 1.39963743 1.99387278
Fe 2.43460614 1.39963467 1.99389751
Fe 1.21758861 3.51683023 2.02586767
Fe 3.65127131 3.51875194 2.02300285
Fe 0.00107493 0.02906061 4.00824695
Fe 2.43471711 0.02908954 4.00824571
Fe 1.21791498 2.12941618 4.01960339
Fe 3.65159506 2.13073974 4.01998302
Fe 1.21838995 0.77731952 6.04275205
Fe 3.65209597 0.77865095 6.03442431
Fe 0.00362058 2.87704072 6.02313843
Fe 2.43318817 2.87712973 6.02313021
Fe 0.00256126 1.52375233 8.07273943
Fe 2.43525933 1.52386589 8.07231633
Fe 1.21896254 3.63318149 8.05518116
Fe 3.65286616 3.61807184 8.01723110
Fe -0.01027911 0.14370475 10.02103676
Fe 2.44961626 0.14354306 10.01954373
Fe 1.21931531 2.27093755 10.08382253
Fe 3.65290130 2.28886962 10.04895665
S 1.22181397 0.79509566 11.70421504
C 2.52460002 3.98939678 14.74988478
C 1.30763069 1.88202032 14.76178983
C 2.52459005 1.17919131 14.75456517
C 1.30761739 3.28667393 14.75536354
C 4.95798208 3.98940215 14.75275639
C 3.74135300 1.88153625 14.74783335
C 4.95796472 1.17919024 14.75786110
C 3.74133872 3.28697428 14.74461747

Graphene on Fe(2x2x6)S_2

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00017676 1.39842270 1.99587964
Fe 2.43369587 1.39849677 1.99437721
Fe 1.21755388 3.51514736 2.02673686
Fe 3.65272393 3.51707852 2.02664642
Fe 0.00412446 0.03112898 4.00619029
Fe 2.43416380 0.02648555 4.00672655
Fe 1.21780956 2.12929056 4.02413051
Fe 3.64902133 2.13405358 4.02399585
Fe 1.22772124 0.76453677 6.03338305
Fe 3.65232602 0.77961323 6.02949605
Fe 0.00176174 2.88443655 6.03113725
Fe 2.42643111 2.86964686 6.03426841
Fe 0.01855044 1.49937847 8.01112801
Fe 2.42786571 1.51322695 8.09047516
Fe 1.22612818 3.61840951 8.09846338
Fe 3.63761502 3.60708558 8.01365308
Fe -0.05427263 0.14532964 9.94925096

Fe 2.36887149 0.16455377 10.19528247
Fe 1.28747493 2.27215259 10.19675369
Fe 3.70803497 2.25148580 9.94483407
S 0.82508276 0.83035107 11.73754790
S 2.83754650 2.94045342 11.73526532
C 2.52728960 4.01393171 14.92767161
C 1.31027327 1.90623271 14.92911886
C 2.52726451 1.20354683 14.92550428
C 1.31028137 3.31126060 14.92777459
C 4.96068117 4.01376636 14.93447258
C 3.74438382 1.90606080 14.93221816
C 4.96064062 1.20360929 14.93600221
C 3.74439384 3.31132365 14.93363748

Graphene on Fe(2x2x6)S_3

Fe 1.21684183 0.70258924 -0.00470693
Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00178241 1.39875451 2.00182165
Fe 2.43545507 1.39931281 1.99915301
Fe 1.21889875 3.51743160 2.04042178
Fe 3.65262464 3.51743298 2.04042624
Fe 0.00275154 0.03854727 4.01938575
Fe 2.43642732 0.03639988 4.02428283
Fe 1.21958798 2.13713935 4.03074427
Fe 3.65331788 2.13714258 4.03076335
Fe 1.22396170 0.78144430 6.05642501
Fe 3.65116201 0.78145297 6.05648897
Fe 0.00390548 2.88158827 6.04429490
Fe 2.43760149 2.87955577 6.04261903
Fe 0.00486009 1.51241202 8.06884080
Fe 2.43848904 1.52563036 8.10994713
Fe 1.22015722 3.61127425 8.02984217
Fe 3.65688059 3.61132764 8.02987947
Fe 0.00591075 0.07284828 10.01201773
Fe 2.43965763 0.09807321 10.08410992
Fe 1.19692477 2.22850259 10.12427658
Fe 3.68219534 2.22836760 10.12388213
S 1.10354751 0.80804248 11.78388614
S 2.44029351 2.92987838 11.79721236
S 3.77668773 0.80824809 11.78384564
C 2.48207770 4.09994232 15.01671288
C 1.26521965 1.99201364 15.01569366
C 2.48204709 1.28931352 15.01703741
C 1.26521972 3.39715600 15.01374942
C 4.91579813 4.09962556 15.01176696
C 3.69901087 1.99199959 15.01450426
C 4.91576239 1.28960983 15.01469191
C 3.69894900 3.39715811 15.01243480

Graphene on Fe(2x2x6)S_4

Fe 1.21684183 0.70258924 -0.00470693

Fe 3.65052362 0.70258924 -0.00470693
Fe -0.00000009 2.81029120 -0.00466931
Fe 2.43368291 2.81029173 -0.00466995
Fe 0.00262230 1.40412580 2.03107761
Fe 2.43630540 1.40412566 2.03107752
Fe 1.21907795 3.50190597 1.99536165
Fe 3.65275906 3.50190598 1.99536165
Fe 0.00353455 0.01990164 4.02616587
Fe 2.43721777 0.01990167 4.02616585
Fe 1.22034522 2.13282631 4.01056474
Fe 3.65402657 2.13282632 4.01056472
Fe 1.22196475 0.76359847 6.03889551
Fe 3.65564595 0.76359847 6.03889546
Fe 0.00514027 2.87466202 6.03824537
Fe 2.43882353 2.87466202 6.03824533
Fe 0.00636054 1.49380086 8.04173041
Fe 2.44004396 1.49380087 8.04173034
Fe 1.22319891 3.60260445 8.03788285
Fe 3.65688038 3.60260445 8.03788286
Fe 0.00846797 0.10686004 10.08979161
Fe 2.44215128 0.10686016 10.08979142
Fe 1.22531380 2.21497744 10.09116467
Fe 3.65899553 2.21497746 10.09116466
S 1.22574453 0.80020266 11.82333075
S 2.44258828 2.90826619 11.82464874
S 3.65942709 0.80020265 11.82333080
S 0.00890533 2.90826577 11.82464744
C 2.49777536 4.07090775 15.05038089
C 1.28093151 1.96320976 15.05034309
C 2.49776503 1.26051893 15.05061007
C 1.28091918 3.36821775 15.05066564
C 4.93145328 4.07090848 15.05038091
C 3.71461857 1.96321071 15.05034292
C 4.93144286 1.26051819 15.05061009
C 3.71460623 3.36821685 15.05066551

Fe_{13}

Fe 2.11738288 2.11732818 2.11721463
Fe 4.12509514 2.11731364 0.87645130
Fe 4.12505427 2.11731685 3.35810198
Fe 0.10964792 2.11732887 0.87640951
Fe 0.10970877 2.11732097 3.35810761
Fe 0.87642997 4.12504154 2.11716220
Fe 3.35813651 4.12507990 2.11716618
Fe 0.87642290 0.10963112 2.11715164
Fe 3.35816217 0.10958553 2.11717191
Fe 2.11738038 0.87635378 4.12478097
Fe 2.11737733 3.35816474 4.12481135
Fe 2.11734922 0.87633978 0.10968880
Fe 2.11734112 3.35818920 0.10966575

Fe_{12}

Fe 3.90852518 4.01727492 5.70613343

Fe 6.12482566 4.01698532 6.41551537
Fe 3.98129390 4.01743534 3.22468485
Fe 1.80693956 4.01719546 4.33819896
Fe 3.28548950 6.05330372 4.38163774
Fe 4.58010139 6.14432333 6.36970258
Fe 3.28577401 1.98138578 4.38164847
Fe 4.58049721 1.88999806 6.36956093
Fe 2.08105411 2.70255061 6.29630870
Fe 2.08073014 5.33160159 6.29618907
Fe 5.67815020 2.75910572 4.45193226
Fe 5.67796631 5.27556604 4.45215544

$Fe_{12}S$

Fe 3.91637103 4.51764282 4.85728275
Fe 6.03851406 4.51842281 5.89140739
S 3.84722771 4.51736462 7.16123346
Fe 3.98636289 4.51767618 2.52931783
Fe 1.77763677 4.51849977 3.73642074
Fe 3.27816527 6.58355407 3.78294720
Fe 4.55249786 6.56336745 5.84730689
Fe 3.27654304 2.45233437 3.78273945
Fe 4.55404188 2.47236581 5.84735134
Fe 2.14812664 3.25135078 5.77212273
Fe 2.14717714 5.78238263 5.77222373
Fe 5.70339515 3.24012778 3.85623166
Fe 5.70445210 5.79356865 3.85625066

Fe_{13} with nanocap(5,0)

Fe 3.95018047 4.01021334 5.37777209
Fe 6.09004860 3.97218024 6.40581418
Fe 3.96358522 4.00789920 7.66021452
Fe 3.94303070 4.01193410 2.94902470
Fe 1.84957779 4.04632921 4.24583141
Fe 3.33059454 6.01554429 4.24073238
Fe 4.64922013 6.02785026 6.41649423
Fe 3.26347253 2.02824830 4.23757679
Fe 4.57863846 1.96774376 6.41268911
Fe 2.20703948 2.78588815 6.42770786
Fe 2.25092306 5.29280418 6.43005496
Fe 5.62168282 2.74917229 4.22765667
Fe 5.66324423 5.21568382 4.22967634
C 4.63733266 5.95167246 8.41533203
C 6.02351674 3.97051603 8.40503658
C 2.32500988 5.24550010 8.42832411
C 2.28180232 2.82829240 8.42605357
C 4.56748820 2.04008163 8.41162482
C 5.57458398 5.12793755 9.17816273
C 3.40027453 5.87759181 9.19188153
C 2.01535558 4.04132624 9.19825529
C 3.33381554 2.15680022 9.18835666
C 5.53347866 2.82838405 9.17597172
C 3.62005703 5.18094575 10.45369107
C 2.74979459 4.02700056 10.45765964

C 4.98643175 4.70983253 10.44509178
C 4.96060737 3.26471669 10.44373662
C 3.57827834 2.84268485 10.45151077

Fe_{13} with nanocap(3,3)

Fe 7.57143192 7.43358886 10.95354870
Fe 9.89988070 7.60854720 11.88970848
Fe 7.89330738 7.40263086 13.24260598
Fe 7.47332286 7.37333070 8.55837323
Fe 5.34349167 7.33358039 9.97982138
Fe 6.71645812 9.33466003 9.78300672
Fe 8.13864007 9.55517263 11.95000130
Fe 6.87002411 5.48108938 9.97305932
Fe 8.58609493 5.47960874 11.83013700
Fe 5.73815620 6.41331741 12.30989505
Fe 5.87912893 8.78870971 12.05866479
Fe 9.37384382 6.43622079 9.68517390
Fe 9.17760001 8.84279630 9.83506093
C 5.22149086 7.78132268 13.81943636
C 5.77325703 9.10304515 13.88462553
C 6.77715285 5.48068943 13.74989711
C 5.52363446 7.15067874 15.10011409
C 6.35114300 5.96367563 15.06158201
C 8.22890357 5.42117784 13.73996824
C 9.67672261 8.20373872 13.78587607
C 9.30539527 7.41828255 14.98916744
C 8.65383576 6.09955805 14.98459721
C 8.75804111 9.34393701 13.79667907
C 6.53610217 9.25939535 15.10256310
C 7.98085233 9.32503327 15.03442954
C 6.20010014 8.11862761 15.94924273
C 8.52061680 8.27026362 15.89226995
C 7.42523684 7.51228762 16.40109869
C 7.51382303 6.16681651 15.90425125

Fe_{12} with nanocap(5,0)

Fe 3.95371878 4.01044317 5.48843885
Fe 6.04604789 3.97943509 6.47140546
Fe 3.94110615 4.01317028 3.00762286
Fe 1.85817976 4.02706736 4.29886828
Fe 3.31580617 6.00325187 4.29357352
Fe 4.63198353 5.98349668 6.48303713
Fe 3.28723999 2.02977871 4.28854477
Fe 4.57664362 2.01605395 6.47701203
Fe 2.25452537 2.80721245 6.49183396
Fe 2.28869950 5.25966021 6.49486093
Fe 5.62911724 2.77145279 4.27710916
Fe 5.64638259 5.22793664 4.28025308
C 4.67766382 5.99942837 8.40336642
C 6.08801382 3.95069780 8.39179539
C 5.58362374 5.10921435 9.11048527
C 2.29374642 5.29324223 8.41592156
C 3.42186711 5.87465242 9.12439552

C 2.23063222 2.80858440 8.41269592
C 2.02666046 4.05596755 9.12993309
C 4.57638861 1.97917279 8.39758943
C 3.32833335 2.16831632 9.11884453
C 5.52728664 2.81738018 9.10791755
C 3.63566241 5.17447571 10.38634524
C 2.76198763 4.03588833 10.39036003
C 4.99153724 4.69404965 10.37687831
C 4.95679952 3.25853808 10.37701399
C 3.57860540 2.85233028 10.38187630

Fe_{12} with nanocap(3,3)

Fe 7.44441849 7.48266653 11.05254997
Fe 9.54758394 7.54072267 12.09404740
Fe 7.46264112 7.44555372 8.53093630
Fe 5.36778257 7.37726355 9.84732551
Fe 6.79994166 9.42304147 9.76330809
Fe 8.11098659 9.49206952 12.07872791
Fe 6.77765417 5.49745588 9.86519954
Fe 8.24039966 5.51628416 11.99412271
Fe 5.79937550 6.29249235 12.23516706
Fe 5.78508407 8.84482155 11.94103879
Fe 9.14783180 6.27967923 9.81683552
Fe 9.14124579 8.72961369 9.89258080
C 5.37752140 7.79274583 13.63683608
C 5.88598730 9.12848815 13.76602665
C 7.06887226 5.44346425 13.67040634
C 5.66180669 7.12577040 14.89555242
C 6.50744036 5.94722314 14.91224152
C 8.49205711 5.49074684 13.82529492
C 9.65927579 8.19707417 13.91029610
C 9.37589030 7.44733973 15.11316926
C 8.81104001 6.12232563 15.07750951
C 8.82592045 9.34651759 13.88256768
C 6.57258843 9.24641444 15.02601948
C 8.00894944 9.35129813 15.07843105
C 6.19526493 8.08696966 15.83195300
C 8.52018871 8.29193674 15.95286831
C 7.40719966 7.50315496 16.35315554
C 7.57568640 6.15944304 15.86150977

Fe_{12}S Top with nanocap(5,0)

Fe 3.88622829 3.98369833 5.15437164
Fe 6.07263761 3.97864438 6.39949981
S 3.93347630 3.99271203 7.29984819
Fe 3.84675876 4.00450343 2.92843216
Fe 1.71893522 4.10745897 4.33037193
Fe 3.23840441 6.05451897 4.26167087
Fe 4.60563388 6.03377468 6.42948856
Fe 3.17498536 2.03805409 4.21444084
Fe 4.54786054 1.93211051 6.42556451
Fe 2.15341235 2.75255027 6.48249533
Fe 2.19701671 5.29859068 6.49145634

Fe 5.62117897 2.76815439 4.24186400
Fe 5.59494246 5.26310990 4.20777687
C 4.65903851 6.03309983 8.43854563
C 6.12477572 3.95968742 8.40167594
C 5.59002803 5.12369347 9.12595157
C 2.23379460 5.28455920 8.49589828
C 3.39785332 5.87026421 9.17942883
C 2.19982319 2.74594844 8.48959546
C 2.01111752 4.01617103 9.20840489
C 4.60232097 1.92735420 8.43138998
C 3.34575100 2.12356102 9.17166536
C 5.55755383 2.80865262 9.12204753
C 3.64939505 5.14941512 10.42236563
C 2.79087559 4.00204588 10.44064903
C 5.00557971 4.68775777 10.38950426
C 4.98579854 3.25475849 10.38740879
C 3.61695621 2.83097693 10.41844772

$Fe_{12}S$ Top with nanocap(3,3)

Fe 7.52094307 7.50710608 10.76816153
Fe 9.73899691 7.62829089 11.97032661
S 7.49457778 7.64415677 12.90797890
Fe 7.49525298 7.53304622 8.50910388
Fe 5.37318859 7.37152380 9.90852349
Fe 6.69840661 9.50020189 9.98455722
Fe 8.28854739 9.51158081 12.00210813
Fe 6.93129236 5.42035961 9.84461911
Fe 8.42368492 5.58245033 12.00317400
Fe 6.05371279 5.94454654 12.08325886
Fe 5.68098143 8.43907604 12.15563410
Fe 9.28280582 6.31565736 9.73414146
Fe 9.22179639 8.81537284 9.78216876
C 5.03892695 7.95350528 13.90886210
C 5.68223604 9.20143059 13.91371508
C 6.82674566 5.29025281 13.83359971
C 5.53066009 7.19480171 15.04973715
C 6.35071888 5.99191873 15.01869244
C 8.28477482 5.29400438 13.88944162
C 9.75919036 8.18468490 13.87186304
C 9.35444815 7.39374407 15.02610014
C 8.68882617 6.08843731 15.03430956
C 8.93427952 9.40180685 13.86458898
C 6.59495410 9.28698131 15.04738715
C 8.05885421 9.35106738 15.02603519
C 6.24083563 8.15531897 15.89577559
C 8.55061471 8.27209394 15.87434726
C 7.43825323 7.54905214 16.39201412
C 7.50985096 6.22205785 15.87946636

$Fe_{12}S$ Edge with nanocap(5,0)

Fe 4.06688461 4.00636384 5.28515425
Fe 3.90838297 4.00559142 7.59081572
Fe 3.65093039 4.01779380 2.90359431

Fe 1.78956331 4.04840564 4.36998219
Fe 3.30879453 6.10192925 4.30468670
Fe 4.80609482 5.91409656 6.44322695
Fe 3.23582667 1.94222291 4.29645106
Fe 4.73282302 2.06762844 6.43623038
Fe 2.29517735 2.72430986 6.37262725
Fe 2.34350655 5.34833819 6.37761797
Fe 5.41733956 2.69223705 3.95991403
Fe 5.46270463 5.27568578 3.96358843
S 6.23452772 3.95959457 6.84475506
C 4.68276817 5.93967470 8.44303172
C 6.08852610 3.95982546 8.62308377
C 5.58992705 5.14100537 9.28823167
C 2.34444989 5.26516319 8.34263115
C 3.40695918 5.87494190 9.15141403
C 2.29561275 2.80410706 8.33781671
C 2.02263192 4.03918161 9.08815580
C 4.60522962 2.03809927 8.43498411
C 3.33286937 2.14988902 9.14409931
C 5.54322046 2.79687801 9.28339802
C 3.54512269 5.17899970 10.42248555
C 2.67709499 4.02364307 10.37703183
C 4.90108849 4.70475005 10.48995299
C 4.87233587 3.25468836 10.48678066
C 3.49851907 2.83432117 10.41801585

Fe_{12}S Edge with nanocap(3,3)

Fe 7.44627465 7.66610035 11.04567593
Fe 9.81779772 7.63525911 11.89672179
Fe 7.79173300 7.69220789 13.32752807
Fe 7.32823205 7.37561724 8.60400106
Fe 5.36079253 7.72574921 10.26848979
Fe 7.06165053 9.49376225 9.46400880
Fe 8.35882596 9.68423202 11.80940997
Fe 6.65226608 5.62884976 10.08640631
Fe 8.38114316 5.62156369 11.94777908
Fe 5.98667396 6.00421735 12.39500794
S 6.00556621 9.31390910 11.95103673
Fe 9.13885487 6.36370853 9.76968437
Fe 9.27883951 8.72850786 9.72908013
C 5.29121094 7.27144975 13.73786949
C 5.82138021 8.59986022 13.57762580
C 6.79339672 5.24367379 13.98332856
C 5.51716527 6.92907016 15.12819156
C 6.37533512 5.78426519 15.27040723
C 8.19566307 5.51295928 13.85564889
C 9.70924447 8.20756684 13.79906158
C 9.28705479 7.49269326 15.01494303
C 8.67162924 6.16584253 15.07340361
C 8.82463791 9.40362354 13.71173248
C 6.46866793 9.05120975 14.82622229
C 7.92228313 9.29677263 14.87171708
C 6.13806762 8.05732235 15.82349449
C 8.46262590 8.36289244 15.86672874

C 7.38345182 7.59107545 16.38624712
C 7.55335250 6.20664556 16.01123297

$Fe_{12}S$ Bottom with nanocap(5,0)

Fe 3.81329831 4.00834053 5.01398152
Fe 3.90588551 4.00405011 7.50491794
Fe 1.52423376 4.02482303 4.55752505
Fe 3.10630511 6.16281245 4.48500708
Fe 4.47466576 6.06088039 6.40061836
Fe 3.02435401 1.84310323 4.50695504
Fe 4.41294710 1.92756517 6.39782164
Fe 2.06326205 2.74469012 6.48375970
Fe 2.10705066 5.31988193 6.47309361
Fe 5.63395907 2.50136956 4.45347619
Fe 5.77788563 5.47250925 4.54380917
Fe 6.01185733 3.95284951 6.34139974
S 5.10334970 4.08110194 2.99866585
C 4.62128523 5.96105410 8.34463724
C 6.01277041 3.97369675 8.29262046
C 5.59100170 5.13732040 9.06824776
C 2.31244988 5.24927903 8.43171297
C 3.40976439 5.88913758 9.15459306
C 2.27406799 2.81322175 8.43781918
C 2.04649378 4.03688632 9.20214705
C 4.56193089 2.03381778 8.34849631
C 3.35401496 2.14451698 9.15953974
C 5.55597628 2.82718473 9.07265665
C 3.68154195 5.18362031 10.40001037
C 2.81633596 4.02731853 10.43547355
C 5.04687474 4.71742450 10.34555244
C 5.02559659 3.26754901 10.34966334
C 3.64697409 2.84486288 10.40399300

$Fe_{12}S$ Bottom with nanocap(3,3)

Fe 7.47282265 7.36135140 10.61390305
Fe 9.77936257 7.38477582 11.89187998
Fe 7.65152731 7.58346752 13.07070611
S 8.16765225 8.22822225 8.48528171
Fe 5.07611398 7.22441206 10.23153995
Fe 6.64609856 9.36569461 9.78864650
Fe 8.10521346 9.55043088 11.80691451
Fe 6.60057368 5.23929695 10.33386943
Fe 8.41529254 5.48070350 11.89172996
Fe 5.79716505 6.24740047 12.33856064
Fe 5.75845799 8.72493391 11.87398429
Fe 9.39542140 6.52715331 9.67400511
Fe 9.54188576 8.91631136 10.08166682
C 5.29144908 7.53898372 13.83842877
C 5.89082328 8.84198579 13.75219887
C 6.72779469 5.45899962 13.89737204
C 5.53779791 7.07922482 15.20053555
C 6.35933704 5.90116060 15.23245643
C 8.15481851 5.55967273 13.78600230

C 9.58813108 8.11716622 13.68598740
C 9.32819783 7.45217221 14.96959042
C 8.67059022 6.15291361 15.02461854
C 8.73406390 9.29689225 13.65321917
C 6.57395798 9.16793311 14.99138603
C 8.02135061 9.32863475 14.94001456
C 6.23342564 8.13687964 15.94599955
C 8.59563161 8.35040898 15.84676546
C 7.48662793 7.58430910 16.37642560
C 7.58214578 6.20879184 15.97797104

Fe_{13} with CNT(5,0)

Fe 3.92058494 4.51171304 4.92409581
Fe 6.04501438 4.56005413 5.96803054
Fe 3.90691359 4.50754048 7.41457767
Fe 3.95850732 4.51865660 2.49607548
Fe 1.83178306 4.47101892 3.77554912
Fe 3.23720901 6.49853524 3.78928523
Fe 4.51760892 6.55444962 5.96643325
Fe 3.31847006 2.50392198 3.78242958
Fe 4.61432407 2.49610340 5.96150490
Fe 2.21575169 3.21757477 5.95643923
Fe 2.15535153 5.71789021 5.95941689
Fe 5.65982793 3.30815189 3.80214749
Fe 5.61055085 5.78899352 3.80658403
C 5.93790726 4.56580759 7.93290658
C 4.58865877 2.59158339 7.92782331
C 5.59392465 3.35090472 8.68774684
C 4.47606235 6.45859153 7.93219215
C 5.52346044 5.75706957 8.69036019
C 2.22557679 5.65317504 7.92693403
C 3.21364632 6.43371616 8.68734200
C 2.29524421 3.26462100 7.92423858
C 1.85724171 4.44616984 8.68284983
C 3.32735708 2.54135361 8.68306760
C 5.52530885 5.75921056 10.09610402
C 5.59650687 3.34644864 10.09345544
C 5.93065359 4.56314108 10.81658050
C 3.20901393 6.43734026 10.09328623
C 4.47018988 6.45339354 10.81672241
C 1.84920012 4.44396182 10.08900826
C 2.22187404 5.64847103 10.81284394
C 3.32386918 2.53414025 10.08907691
C 2.29227691 3.26164904 10.81033066
C 4.58406480 2.59044911 10.81260961
C 4.47426152 6.47274988 12.22228054
C 5.95067652 4.56264924 12.22196340
C 5.51798651 5.75388247 12.94048630
C 2.20183537 5.65894039 12.21869834
C 3.20648772 6.42985353 12.93883013
C 2.27341725 3.24647208 12.21616758
C 1.84968697 4.44034379 12.93520746
C 4.59000632 2.56860379 12.21819511
C 3.32229554 2.53501572 12.93476529

C 5.58967961 3.34657716 12.93807137
C 3.19893744 6.44512470 14.35936894
C 5.53062770 5.76352462 14.36088977
C 4.44034329 6.36408085 15.08872877
C 1.83052103 4.43813268 14.35595874
C 2.28980923 5.59375206 15.08590078
C 3.31626794 2.51631593 14.35534682
C 2.35817090 3.31040962 15.08361105
C 5.60326663 3.33524560 14.35841786
C 4.55076384 2.66951614 15.08493757
C 5.83760347 4.55685756 15.08817196
C 2.88487282 5.18607063 16.35659195
C 2.92776307 3.75017478 16.35520005
C 4.23718585 5.67066131 16.35846977
C 5.11607161 4.53411521 16.35817950
C 4.30663403 3.34724609 16.35603977

Fe_{13} with CNT(3,3)

Fe 7.51176113 7.39897455 7.84620464
Fe 9.69780783 7.66791013 8.86552503
Fe 7.60776563 7.41180813 10.22642229
Fe 7.38510121 7.35156390 5.47852604
Fe 5.36682832 7.28834786 6.88059137
Fe 6.50214601 9.36004723 6.97683766
Fe 8.09104325 9.47146221 8.85586390
Fe 7.10862704 5.31109885 6.74378605
Fe 8.48871184 5.45471507 8.93522675
Fe 6.06105109 5.89468652 8.87326070
Fe 5.69875435 8.43909543 9.22006634
Fe 9.36707595 6.28487488 6.79430926
Fe 8.97978745 8.74746372 6.61525685
C 5.48186364 7.07040841 10.76011505
C 6.23869664 5.88498879 10.78476250
C 8.96640569 5.93506549 10.78161972
C 9.59699187 7.21616737 10.78253082
C 6.57583271 9.33476077 10.78809152
C 7.97434172 9.43382545 10.79317674
C 5.31912406 7.73725542 12.04643455
C 5.94736099 9.02855788 12.06240105
C 6.88217305 5.47498766 12.02067519
C 5.39314317 6.97845485 13.25330348
C 6.21389192 5.78257949 13.24549160
C 8.31500745 5.53944604 12.02362875
C 9.50666681 7.97578683 12.02493375
C 8.92416358 5.94190730 13.25928408
C 9.56125054 7.24368646 13.26096163
C 8.68769128 9.15335322 12.03128129
C 6.59122119 9.41618763 13.27320139
C 8.03946185 9.49006147 13.26237308
C 5.36235826 7.69587470 14.50034659
C 5.99890066 8.98820449 14.51060724
C 6.86636855 5.45755772 14.48445850
C 5.38331337 6.94774730 15.72482829
C 6.19228890 5.74693324 15.71604238

C 8.30495361 5.54796387 14.48803565
C 9.49385539 7.96570724 14.49648547
C 8.93629972 5.93017107 15.71976185
C 9.57245985 7.22352966 15.72433375
C 8.68988285 9.16151338 14.50116332
C 6.59944285 9.41674394 15.74015576
C 8.04419234 9.50884192 15.73453792
C 5.34227924 7.68394771 16.94865298
C 5.98514491 8.98966852 16.95666816
C 6.86486677 5.41710964 16.93643934
C 5.60522017 7.07758251 18.22404687
C 6.41007486 5.87663275 18.21654574
C 8.31781063 5.50996098 16.93999060
C 9.52320614 7.95966850 16.95135647
C 9.34972504 7.32317092 18.22339278
C 8.71109708 6.02470044 18.21769701
C 8.71024042 9.16731969 16.95529646
C 6.61989222 9.14082458 18.23590669
C 8.06267692 9.23613281 18.23357091
C 6.23312822 8.04517668 19.09521081
C 8.59315971 8.19982104 19.09382073
C 7.46165069 7.43867162 19.54687551
C 7.55132097 6.08155544 19.08379810

Fe_{12} with CNT(5,0)

Fe 3.92075022 4.51092283 4.97354709
Fe 5.96872266 4.54653547 6.02585478
Fe 3.93230226 4.51446156 2.48457431
Fe 1.83868556 4.48874824 3.78158103
Fe 3.25755484 6.48901884 3.78805289
Fe 4.51526481 6.47214117 6.02416635
Fe 3.30200995 2.52128735 3.78414081
Fe 4.58604821 2.56985444 6.02038978
Fe 2.27978852 3.27374248 6.01533879
Fe 2.23567232 5.68471913 6.01759099
Fe 5.62729191 3.30431272 3.79246555
Fe 5.60001036 5.75800298 3.79483975
C 5.92457513 4.56846452 7.94437444
C 4.59197487 2.60781220 7.93952589
C 5.57549621 3.37062655 8.68049957
C 4.47129191 6.44166331 7.94265217
C 5.50092435 5.74069429 8.68240212
C 2.24111465 5.63781382 7.93680184
C 3.22370857 6.40185599 8.67790174
C 2.31598016 3.26891375 7.93489445
C 1.89106301 4.44052079 8.67326551
C 3.34452354 2.56689684 8.67493790
C 5.50869428 5.74816942 10.09330974
C 5.58410087 3.36175216 10.09143211
C 5.93796236 4.56686645 10.81955433
C 3.21571192 6.41364826 10.08883223
C 4.47017274 6.45801906 10.81799323
C 1.87414219 4.43863106 10.08425095
C 2.21814987 5.64634549 10.81247771

C 3.33781303 2.55227336 10.08585576
C 2.29387886 3.25377715 10.81066481
C 4.59281325 2.58663398 10.81501036
C 4.47218273 6.47471261 12.22159429
C 5.95360712 4.56658651 12.22315550
C 5.51955903 5.75945031 12.94082464
C 2.19976634 5.65544866 12.21615504
C 3.20207469 6.43157622 12.93654802
C 2.27656510 3.24116810 12.21436079
C 1.84666796 4.43526659 12.93213827
C 4.59647706 2.56821202 12.21866977
C 3.32642958 2.52934629 12.93368385
C 5.59639203 3.34769738 12.93903075
C 3.19424231 6.44392306 14.35597100
C 5.52790724 5.76724600 14.36022195
C 4.43533312 6.36621363 15.08688261
C 1.82959904 4.43361001 14.35161339
C 2.28547040 5.59091822 15.08186440
C 3.31972923 2.51447211 14.35312535
C 2.35848861 3.30669661 15.08020384
C 5.60543852 3.33863594 14.35846456
C 4.55341385 2.67020224 15.08418611
C 5.83699045 4.56108699 15.08835335
C 2.88062469 5.18426215 16.35436210
C 2.92657371 3.74882463 16.35327116
C 4.23165287 5.67146772 16.35749979
C 5.11257627 4.53708157 16.35845330
C 4.30586845 3.34881735 16.35581233

Fe_{12} with CNT(3,3)

Fe 7.22967207 7.25585356 8.14281078
Fe 9.42054960 7.36087938 9.05100615
Fe 7.16511555 7.20001087 5.64390735
Fe 5.10819302 7.34130415 6.95890625
Fe 6.57132298 9.24209428 6.94229883
Fe 8.04076724 9.29817756 9.04145271
Fe 6.62754543 5.21477077 6.96687767
Fe 8.00035239 5.39402704 9.26150980
Fe 5.41211319 5.95993550 8.90598796
Fe 5.71727746 8.59481818 9.24956886
Fe 8.90004371 5.98349127 6.95491105
Fe 8.91383784 8.45395778 6.85494052
C 5.75354028 7.07908230 10.60013944
C 6.57395731 5.92623569 10.60561827
C 9.20554181 6.19105455 10.77347501
C 9.82464489 7.41864764 10.88418833
C 6.86706576 9.48103147 10.75818445
C 8.22962944 9.66266360 10.87347312
C 5.59433070 7.74429510 11.88712693
C 6.19136290 9.02547021 11.96095727
C 7.14344362 5.56582958 11.89799743
C 5.57763253 6.98106398 13.10489724
C 6.41104577 5.80885470 13.11067545
C 8.54908326 5.70979072 11.97749297

C 9.70278069 8.15485243 12.10783060
C 9.09662176 6.08208801 13.25606361
C 9.70033639 7.38462268 13.32888756
C 8.87962757 9.31260292 12.10195965
C 6.71729338 9.42861853 13.23916951
C 8.14549684 9.57107280 13.31777239
C 5.44841174 7.67140414 14.35482277
C 6.05383496 8.97907545 14.42722590
C 7.01443431 5.46858653 14.36610795
C 5.43271317 6.89400647 15.56245716
C 6.26904716 5.71759106 15.56837210
C 8.44804553 5.61118438 14.44426988
C 9.57805879 8.06497122 14.58349723
C 9.00372027 5.97777390 15.71553612
C 9.60675998 7.28852942 15.78907757
C 8.74208057 9.24067687 14.57744211
C 6.57668613 9.39222681 15.69795005
C 8.01251224 9.53141235 15.77746036
C 5.30883595 7.59869011 16.80353120
C 5.91258050 8.91812837 16.87472135
C 6.88763635 5.37764582 16.81507567
C 5.51647543 6.96738557 18.07603587
C 6.35332882 5.79020852 18.08204777
C 8.33180166 5.51458513 16.89233439
C 9.46378161 7.99080500 17.02859480
C 9.24111659 7.31876432 18.27830149
C 8.64198315 6.00671601 18.20502234
C 8.62270529 9.17414949 17.02251007
C 6.47288834 9.05837314 18.18921519
C 7.90863327 9.19337661 18.26851994
C 6.07330187 7.93015844 19.00267379
C 8.42214417 8.15201582 19.13272330
C 7.28881655 7.34851751 19.50730653
C 7.44101873 6.00600594 19.01257167

$Fe_{12}S$ Top with CNT(5,0)

Fe 3.91584273 4.50840709 4.64499396
Fe 6.04841160 4.56613044 6.01278507
Fe 3.94421239 4.51692462 2.42431639
Fe 1.77500814 4.45388673 3.81875104
Fe 3.21223577 6.54255606 3.82739301
Fe 4.51850490 6.55460975 6.01107862
Fe 3.31839433 2.44430401 3.82321893
Fe 4.63093017 2.49600012 6.00761400
Fe 2.22190305 3.20441031 6.00263929
Fe 2.15267250 5.71368243 6.00468687
Fe 5.70138289 3.29117570 3.83090477
Fe 5.63707468 5.81935047 3.83384682
S 3.91121565 4.50594250 6.78488950
C 6.00063722 4.56583190 7.97155106
C 4.61267398 2.53485037 7.96635244
C 5.58384049 3.35914817 8.69658724
C 4.49741996 6.51307097 7.96989378
C 5.51463946 5.74521817 8.69875854

C 2.18100425 5.68544184 7.96352888
C 3.22381616 6.41660458 8.69403925
C 2.25211421 3.22667797 7.96135527
C 1.87719713 4.44554890 8.68901009
C 3.33576458 2.55576416 8.69055066
C 5.51152793 5.74415671 10.10845724
C 5.58080563 3.35761858 10.10631436
C 5.93662466 4.56158432 10.83558183
C 3.22027953 6.41542156 10.10392189
C 4.47449545 6.45539541 10.83417319
C 1.87362784 4.44401704 10.09898220
C 2.22149586 5.65019602 10.82851065
C 3.33244587 2.55410486 10.10045930
C 2.29088051 3.25859657 10.82638018
C 4.58699773 2.58598452 10.83069235
C 4.47680001 6.47236819 12.23575024
C 5.95280557 4.56088042 12.23705742
C 5.52868013 5.75950792 12.95494184
C 2.20271948 5.65952065 12.23016882
C 3.20422185 6.44040142 12.95077926
C 2.27294296 3.24555657 12.22800975
C 1.83815742 4.44026622 12.94609687
C 4.59059840 2.56667110 12.23225806
C 3.31840498 2.52310796 12.94728910
C 5.59927186 3.33839056 12.95275612
C 3.19781041 6.44947174 14.36523840
C 5.53469593 5.76499001 14.36934762
C 4.44299192 6.37329574 15.09651425
C 1.82454273 4.43860393 14.36056774
C 2.28038815 5.60006161 15.09143658
C 3.31272331 2.51116497 14.36171701
C 2.34743143 3.30443460 15.08939078
C 5.60573422 3.33087224 14.36716068
C 4.55141195 2.65868440 15.09316601
C 5.84667238 4.55536651 15.09763335
C 2.88026737 5.18771091 16.35023165
C 2.92233106 3.74896179 16.34888523
C 4.23561475 5.67226171 16.35345383
C 5.11533735 4.53292202 16.35415118
C 4.30358085 3.34422807 16.35134849

$Fe_{12}S$ Top with CNT(3,3)

Fe 7.53730515 7.44893134 7.70706194
Fe 9.72928095 7.59199851 8.93396260
S 7.51398767 7.34712114 9.82956960
Fe 7.43812837 7.36825027 5.43656407
Fe 5.40075661 7.36316057 6.84374748
Fe 6.81728634 9.47715361 6.77331658
Fe 8.26578530 9.50957038 8.91696134
Fe 6.83898559 5.34477143 7.02427922
Fe 8.49199866 5.56667368 8.99206698
Fe 5.82667170 6.31078262 9.12978136
Fe 5.96382885 8.85017162 9.01273344
Fe 9.26375369 6.24888365 6.72255926

Fe 9.18460741 8.72437081 6.63689192
C 5.19305089 6.71720139 10.90331538
C 6.00201088 5.60441680 10.90968825
C 9.13683627 5.83421623 10.85025950
C 9.76962990 7.11322441 10.84628733
C 6.52649082 9.50090148 10.82168563
C 7.92799084 9.68341209 10.83444819
C 5.30523152 7.61177646 12.02445606
C 5.93965522 8.89549111 12.00408014
C 6.89188127 5.38741444 12.02123581
C 5.42776441 6.89769083 13.28648845
C 6.25737511 5.73084651 13.28563903
C 8.32155404 5.52373303 12.01056721
C 9.47143973 7.96985814 11.98609212
C 8.89477960 5.96778981 13.26793379
C 9.49879171 7.26049216 13.25390559
C 8.63853865 9.13770245 11.98080834
C 6.55563824 9.29236359 13.25649507
C 7.97793034 9.41537349 13.24480605
C 5.34601551 7.61672736 14.52119933
C 5.95614535 8.92567508 14.50369040
C 6.90010390 5.40647959 14.52381275
C 5.39073959 6.88529066 15.74975126
C 6.22473994 5.69771096 15.75102064
C 8.33831572 5.53434183 14.51283493
C 9.48081521 7.98373034 14.48862183
C 8.97321319 5.94120640 15.72953580
C 9.58376049 7.25591689 15.71579182
C 8.64921687 9.16262722 14.48364699
C 6.55390820 9.38659011 15.71988559
C 7.99752085 9.51356410 15.70846430
C 5.34531820 7.63843283 16.96354033
C 5.95795851 8.95906012 16.94871238
C 6.91526687 5.40273581 16.96818364
C 5.62882002 7.05517018 18.24336000
C 6.45972113 5.87063426 18.24625071
C 8.36491969 5.53089932 16.95703662
C 9.51437154 8.00729706 16.93177845
C 9.35988041 7.38476623 18.21405634
C 8.75089795 6.07330872 18.22821959
C 8.67738128 9.19833409 16.92767962
C 6.59570908 9.14292952 18.22009998
C 8.03599463 9.26971483 18.20853266
C 6.23821979 8.04881675 19.09877041
C 8.59388438 8.25666735 19.07935706
C 7.48055556 7.47579879 19.54632185
C 7.59898471 6.11036537 19.10361748

$Fe_{12}S$ Edge with CNT(5,0)

Fe 4.08723530 4.51745337 4.88506903
Fe 3.99372894 4.50331822 7.45505241
Fe 3.62511646 4.52600533 2.43886535
Fe 1.80317018 4.45771917 3.92084489
Fe 3.18399385 6.57252437 3.86048583

Fe 4.65470787 6.48527932 5.94986172
Fe 3.30174835 2.43431221 3.83457638
Fe 4.75551236 2.57193744 5.93999465
Fe 2.39462857 3.20116337 5.95768105
Fe 2.32438958 5.72629569 5.96380458
Fe 5.42421432 3.27919273 3.42986265
Fe 5.35301096 5.85790562 3.44930032
S 6.12757475 4.56116786 6.24500000
C 5.96148857 4.55228623 8.02785882
C 4.62716562 2.55107482 7.92460150
C 5.60505612 3.31638982 8.72084696
C 4.52942178 6.48397639 7.93030745
C 5.54582786 5.76747213 8.72394681
C 2.33066173 5.66904599 7.91723115
C 3.26570653 6.50193075 8.69411615
C 2.39129166 3.25208342 7.91397398
C 2.00123217 4.45067929 8.65897650
C 3.36652146 2.46585096 8.69040806
C 5.52630161 5.75380379 10.12894663
C 5.58491663 3.32649687 10.12705892
C 5.89967884 4.54784657 10.84862371
C 3.24167062 6.50325642 10.09072931
C 4.49736596 6.49613767 10.83736859
C 1.96769347 4.44920628 10.07495587
C 2.27366326 5.66385447 10.79645708
C 3.34217674 2.46152061 10.08775175
C 2.33366618 3.25112846 10.79550375
C 4.59544424 2.53270011 10.83562434
C 4.48539714 6.50267509 12.23923720
C 5.90568992 4.54764007 12.25373264
C 5.49786263 5.74930683 12.96598512
C 2.22761538 5.66928068 12.19944353
C 3.20018036 6.47728805 12.94245090
C 2.28782891 3.24392644 12.19908394
C 1.88349964 4.44738914 12.90011312
C 4.58361156 2.52512827 12.23836385
C 3.29883296 2.48563869 12.94281440
C 5.55608623 3.32818662 12.96567315
C 3.17591398 6.48363719 14.35173589
C 5.49085816 5.75787985 14.38576466
C 4.41256978 6.38899923 15.09861681
C 1.83606790 4.44652311 14.32333421
C 2.26358082 5.60707382 15.06154774
C 3.27436336 2.47862343 14.35246326
C 2.31961983 3.30912655 15.06192752
C 5.54926992 3.31967706 14.38614951
C 4.50465442 2.63565785 15.09971937
C 5.77793426 4.54494466 15.11933630
C 2.82849897 5.19704886 16.33521990
C 2.86469063 3.74878428 16.33512822
C 4.18106892 5.66596294 16.34842190
C 5.06408904 4.52768502 16.38124650
C 4.23809620 3.34678121 16.34950410

$Fe_{12}S$ Edge with CNT(3,3)

Fe 7.51779568 7.09721137 7.90027447
Fe 9.62206198 7.11213027 9.02510807
Fe 7.62244169 7.43537215 10.28818295
Fe 7.50685127 7.64969039 5.46349045
Fe 5.29294204 7.55286089 6.94135373
Fe 6.88342533 9.34027766 7.00053282
Fe 8.32189671 9.26082586 8.88413476
Fe 6.39736056 5.71210432 6.09484583
S 7.34405815 4.70387191 7.81177097
Fe 5.79272560 6.01248498 8.94857420
Fe 5.85638037 8.53404755 9.17774217
Fe 9.05043147 5.93457862 6.73280638
Fe 9.34926816 8.33542723 6.87588887
C 5.55870443 7.01378349 10.74203760
C 6.40810182 5.88644289 10.77978226
C 9.15232383 6.18382189 10.84414182
C 9.75667057 7.42072451 10.91164952
C 6.60494057 9.34843669 10.82549552
C 7.99116549 9.49412105 10.83703318
C 5.36748073 7.68357919 12.02362262
C 5.95168756 8.99622567 12.07327155
C 7.07585910 5.50998748 12.00121204
C 5.47532340 6.91348820 13.22507650
C 6.36940780 5.76783335 13.22131381
C 8.51321354 5.66566685 12.02774474
C 9.61634490 8.18994600 12.11971088
C 9.07485381 6.08845254 13.28748305
C 9.64710305 7.42150861 13.33205555
C 8.69393906 9.29480853 12.09628773
C 6.54903454 9.40744299 13.29921933
C 7.99152604 9.57031618 13.31492998
C 5.38931111 7.61479658 14.47700346
C 5.95573841 8.93642587 14.51841902
C 7.02124888 5.47297368 14.46557221
C 5.43013857 6.85387673 15.69520441
C 6.30441742 5.70511259 15.68879415
C 8.45245002 5.64241323 14.50003237
C 9.49965787 8.11953792 14.57472765
C 9.03182750 6.03890209 15.75421775
C 9.59487219 7.36641313 15.79445977
C 8.62981975 9.26432015 14.56752289
C 6.50396180 9.38123739 15.76713006
C 7.93769728 9.55891719 15.79390259
C 5.31360357 7.56960963 16.92805389
C 5.88425478 8.90951549 16.96605966
C 6.96438337 5.39148095 16.91964133
C 5.58148933 6.96091723 18.19820611
C 6.45464032 5.80777545 18.19242090
C 8.41030956 5.56857684 16.95456497
C 9.47737239 8.08289523 17.02449211
C 9.30825769 7.42033902 18.28562046
C 8.74381871 6.09025627 18.24663865
C 8.59716897 9.24338811 17.02372295
C 6.48214141 9.07892508 18.25820515

C 7.91701108 9.25500526 18.28835565
C 6.13945820 7.95032316 19.09559913
C 8.48471044 8.24004276 19.14815898
C 7.38645280 7.40933641 19.57018310
C 7.56335486 6.06934162 19.08787732

$Fe_{12}S$ Bottom with CNT(5,0)

Fe 3.91990571 4.50894728 4.86518099
Fe 3.91090258 4.50590341 7.39050700
Fe 1.84464519 4.46181295 3.72889134
Fe 3.23799453 6.47577981 3.73411316
Fe 4.51567049 6.55927849 5.96989459
Fe 3.33062212 2.51623400 3.72951378
Fe 4.62864950 2.49160542 5.96614641
Fe 2.21914928 3.20287290 5.96077511
Fe 2.14883499 5.71393713 5.96305143
Fe 5.64025555 3.32618183 3.74062503
Fe 5.58273422 5.77454416 3.74265877
Fe 6.05199645 4.56650613 5.97179676
S 3.93580781 4.51414407 2.38107156
C 5.93359195 4.56482829 7.94532125
C 4.59126870 2.59805383 7.94022808
C 5.59748380 3.35087126 8.70019943
C 4.47776976 6.44938173 7.94371148
C 5.52636481 5.75543811 8.70231525
C 2.23591622 5.64714636 7.93758113
C 3.21779602 6.43135820 8.69786147
C 2.30593755 3.26706645 7.93542112
C 1.86204488 4.44445500 8.69289777
C 3.33245119 2.54094613 8.69439715
C 5.52895124 5.75850154 10.10876309
C 5.60036214 3.34547916 10.10658500
C 5.93480387 4.56231706 10.82945156
C 3.21222524 6.43690392 10.10411492
C 4.47359577 6.45391739 10.82805612
C 1.85157214 4.44292681 10.09910276
C 2.22322198 5.64881260 10.82236946
C 3.32731245 2.53265063 10.10067452
C 2.29355356 3.25975510 10.82029265
C 4.58745774 2.58824088 10.82464996
C 4.47654206 6.47277760 12.23316260
C 5.95293454 4.56164490 12.23467001
C 5.51971640 5.75337424 12.95250991
C 2.20274595 5.65935791 12.22727916
C 3.20752066 6.43034869 12.94812523
C 2.27382014 3.24547236 12.22514987
C 1.84938217 4.44038508 12.94324139
C 4.59156089 2.56705530 12.22973668
C 3.32227415 2.53378445 12.94466534
C 5.59084247 3.34514491 12.95048361
C 3.19852868 6.44559192 14.36828138
C 5.53051020 5.76279252 14.37284757
C 4.43913036 6.36372801 15.09912154
C 1.82878118 4.43861496 14.36335073

C 2.28804603 5.59430395 15.09353733
C 3.31429795 2.51563368 14.36484202
C 2.35541949 3.31073033 15.09158478
C 5.60223657 3.33393251 14.37073338
C 4.54791549 2.66879624 15.09584842
C 5.83572574 4.55572068 15.10054897
C 2.88123821 5.18639057 16.36505233
C 2.92342412 3.75051124 16.36388007
C 4.23371506 5.67022957 16.36861564
C 5.11183518 4.53338086 16.36949755
C 4.30205696 3.34703602 16.36649276

$Fe_{12}S$ Bottom with CNT(3,3)

Fe 7.34858439 7.44859775 7.63222179
Fe 9.56322435 7.61088782 8.81226135
Fe 7.53480761 7.51417968 10.14443319
S 8.38626019 6.83198769 5.55004754
Fe 5.09202639 7.51712045 7.09706584
Fe 6.49065963 9.63552806 7.16282241
Fe 8.11272411 9.55900193 8.84104035
Fe 6.98601523 5.30578460 6.90725356
Fe 7.97798047 5.39000351 9.15286664
Fe 5.64954923 6.08775642 8.88153138
Fe 5.65510847 8.62122148 9.19208000
Fe 9.34943583 5.82264023 7.26739749
Fe 9.00482965 8.74824445 6.70841093
C 5.53121912 7.04527028 10.71809866
C 6.34952876 5.88167584 10.72959349
C 8.93919219 6.01667500 10.74783988
C 9.55034545 7.28560316 10.74708214
C 6.57720574 9.38444044 10.78243701
C 7.97355925 9.49139463 10.78793044
C 5.36105703 7.71058926 12.00904716
C 5.95287024 9.01699782 12.04629589
C 6.94473694 5.46728112 11.99227522
C 5.42691686 6.94772638 13.21662514
C 6.26066970 5.75942317 13.20926258
C 8.37230498 5.56033755 12.01270944
C 9.51066508 8.02869967 12.00764228
C 8.98019768 5.97071295 13.23431335
C 9.59071696 7.29059387 13.23473029
C 8.68154652 9.19400232 12.02441496
C 6.57822727 9.41171326 13.26488714
C 8.02699404 9.51381036 13.25721276
C 5.37960924 7.65732155 14.46731572
C 5.99124008 8.95997323 14.49219660
C 6.92295886 5.44626195 14.44712090
C 5.41231385 6.90293536 15.69068024
C 6.23970426 5.71942630 15.67968284
C 8.35930954 5.56290187 14.45910927
C 9.50422348 8.00201500 14.47889600
C 8.97863317 5.94967094 15.69449409
C 9.59158274 7.25500264 15.70505494
C 8.67901412 9.18150727 14.49189671

C 6.58282019 9.38816546 15.72733091
C 8.02102814 9.50875835 15.72678874
C 5.35036820 7.63029741 16.92161533
C 5.96974328 8.94638216 16.94116814
C 6.91294396 5.39278726 16.90099120
C 5.61802452 7.02113410 18.19400235
C 6.44483627 5.83564886 18.18310130
C 8.36212521 5.51332640 16.90912661
C 9.52202281 7.98237281 16.93680639
C 9.35430124 7.33560924 18.20672433
C 8.74074724 6.02766663 18.19315971
C 8.68926345 9.17453657 16.94816195
C 6.59496335 9.10568200 18.22267688
C 8.03569480 9.22556762 18.22488623
C 6.22722596 7.99527904 19.07286397
C 8.58033359 8.19344835 19.08071819
C 7.46191027 7.41019116 19.52935017
C 7.57800826 6.05728772 19.05581771

Fe_{55}

Fe 3.45383220 3.45387878 3.45234591
Fe 5.39899616 3.45402983 2.25071892
Fe 5.39896035 3.45425207 4.65424351
Fe 1.50879940 3.45461872 2.25076598
Fe 1.50875560 3.45479450 4.65417599
Fe 2.25260921 5.39947621 3.45246589
Fe 4.65664516 5.39893410 3.45240687
Fe 2.25206539 1.50890656 3.45237690
Fe 4.65637530 1.50893517 3.45242944
Fe 3.45391570 2.25162445 5.39726037
Fe 3.45414595 4.65628942 5.39722261
Fe 3.45405981 2.25186577 1.50724407
Fe 3.45435799 4.65629419 1.50741150
Fe 7.45618545 3.45289192 0.97925703
Fe 7.48014821 3.45475386 3.45253877
Fe 7.45590975 3.45340573 5.92603410
Fe -0.54941584 3.45405206 0.97995822
Fe -0.57294531 3.45564852 3.45253751
Fe -0.54966218 3.45445456 5.92486477
Fe 0.98076388 7.45790869 3.45218172
Fe 3.45473016 7.48003863 3.45212855
Fe 5.92791570 7.45716247 3.45219308
Fe 0.98052070 -0.54944743 3.45251033
Fe 3.45448190 -0.57271840 3.45239427
Fe 5.92716328 -0.54957315 3.45273302
Fe 3.45352254 0.97915577 7.45496260
Fe 3.45360518 3.45329595 7.47864827
Fe 3.45375847 5.92685330 7.45598075
Fe 3.45369545 0.97951841 -0.55040130
Fe 3.45351853 3.45344394 -0.57450715
Fe 3.45392931 5.92687219 -0.55123529
Fe 5.46704955 2.20883440 6.70923794
Fe 5.46672231 4.69773524 6.70900765
Fe 5.46716492 2.20900385 0.19519860

Fe 5.46688870 4.69752125 0.19557281
Fe 1.44027184 2.20937456 6.70886215
Fe 1.44024533 4.69798401 6.70895411
Fe 1.44019407 2.20925639 0.19577469
Fe 1.44019248 4.69798812 0.19591376
Fe 6.71119901 5.46751492 2.20849472
Fe 6.71133945 5.46747779 4.69616439
Fe 0.19666505 5.46832502 2.20862985
Fe 0.19664077 5.46824681 4.69625747
Fe 6.71098359 1.43997763 2.20880965
Fe 6.71115206 1.44036903 4.69602650
Fe 0.19621410 1.44061499 2.20884040
Fe 0.19631707 1.44109188 4.69591892
Fe 2.21032479 6.71168667 5.46571011
Fe 4.69790971 6.71217985 5.46545324
Fe 2.21002621 0.19529137 5.46516013
Fe 4.69775134 0.19523406 5.46549525
Fe 2.21024092 6.71119145 1.43899710
Fe 4.69826406 6.71168155 1.43898009
Fe 2.20993931 0.19564771 1.43980371
Fe 4.69797755 0.19578701 1.43952123

$Fe_{54}S$

Fe 3.45396041 3.55199791 3.44822688
Fe 5.39903007 4.15387484 2.41167333
Fe 5.39513564 2.95352255 4.50702310
Fe 1.50910092 4.15296685 2.41193240
Fe 1.51328280 2.95277333 4.50675374
Fe 2.25439180 5.23394590 4.43707162
Fe 4.65275914 5.23435856 4.43680003
Fe 2.25211855 1.86749965 2.48220571
Fe 4.65700898 1.86814217 2.48198363
Fe 3.45509236 1.54302677 4.54830113
Fe 3.45396545 3.62191343 5.77522853
Fe 3.45397203 3.48275496 1.17207298
Fe 3.45362382 5.56566255 2.36876633
Fe 7.45842870 4.79078856 1.30823876
Fe 7.47530664 3.54653369 3.46238796
Fe 7.48105026 2.30978716 5.62737179
Fe -0.55012040 4.78929319 1.30802382
Fe -0.56752464 3.54447192 3.46245393
Fe -0.57444033 2.30731268 5.62542884
Fe 0.96375135 7.04186391 5.48151151
Fe 3.45261885 7.04640047 5.46619226
Fe 5.94055899 7.04310937 5.48176989
Fe 0.97878567 0.08530031 1.44719752
Fe 3.45393346 0.05862298 1.44422869
Fe 5.92835992 0.08538637 1.44620331
Fe 3.45644623 -0.61811124 5.71167902
Fe 3.45541145 1.48004177 6.90021149
S 3.44995100 3.68416531 8.01049561
Fe 3.45604357 3.41047893 -1.23191656
Fe 3.45343812 5.57187286 -0.03540765
Fe 3.45417982 7.69671079 1.21836191

Fe 5.47244466 0.84132698 5.65224506
Fe 5.52062405 2.98257445 6.85843284
Fe 5.47502910 4.10525757 0.00846693
Fe 5.47068455 6.26350884 1.25446091
Fe 1.43842026 0.84136972 5.65162997
Fe 1.38558311 2.98096353 6.85725154
Fe 1.43274207 4.10399334 0.00828509
Fe 1.43640057 6.26287730 1.25469721
Fe 6.70317477 5.92252342 3.38945038
Fe 6.71543941 4.67725149 5.53823336
Fe 0.20378875 5.92117260 3.38904808
Fe 0.19047049 4.67563827 5.53725569
Fe 6.71747226 2.43023813 1.37307334
Fe 6.71426393 1.19573141 3.53057959
Fe 0.19076739 2.42961782 1.37305200
Fe 0.19539302 1.19365754 3.53079448
Fe 2.17482108 5.41088230 6.78246736
Fe 4.72927299 5.41144017 6.78271914
Fe 2.21782253 -0.27430032 3.57607869
Fe 4.69152381 -0.27321527 3.57523453
Fe 2.20400972 7.37340279 3.34476475
Fe 4.70284503 7.37421751 3.34464007
Fe 2.20558745 1.72980670 0.08090470
Fe 4.70283300 1.73005373 0.08113604

$Fe_{52}S_3$

Fe 3.44085395 3.59849283 3.40691485
Fe 5.41559022 4.16328855 2.39892320
Fe 5.36018221 2.98825563 4.53604870
Fe 1.51628558 4.15266969 2.31108032
Fe 1.49775240 2.98171909 4.42029482
Fe 2.21025342 5.32398886 4.18526934
Fe 4.66206707 5.27444393 4.35282725
Fe 2.26287292 1.87913430 2.46543112
Fe 4.65905903 1.89333434 2.51067515
Fe 3.45038638 1.60449855 4.57501902
Fe 3.22414392 3.96903148 5.81614279
Fe 3.48975605 3.46549619 1.15345174
Fe 3.48369361 5.57731090 2.26694197
Fe 7.51397692 4.79103608 1.35654808
Fe 7.48790198 3.62463905 3.50236136
Fe 7.14390377 2.44948880 5.79227886
Fe -0.52654765 4.79457853 1.21787442
Fe -0.54174105 3.66753131 3.44079507
Fe -0.56510568 2.48479595 5.60624779
Fe 1.00236456 7.03019960 5.37709324
Fe 3.40244347 6.85165936 5.50919125
Fe 5.81759857 7.10015631 5.46716077
Fe 0.98363336 0.06369597 1.49167874
Fe 3.43762057 0.07917235 1.43048444
Fe 5.95873356 0.07376366 1.54251316
Fe 3.44121468 -0.24055615 5.85861078
S 2.65184994 1.02069625 7.62031308
Fe 4.48376225 2.23204142 6.76446821

Fe 3.53695101 3.32696685 -1.26545393
Fe 3.48169230 5.53867075 -0.11226568
Fe 3.47402295 7.69103735 1.12205682
Fe 5.67218372 0.57383080 5.45790025
S 6.21676769 3.62122082 7.54815570
Fe 5.50655624 4.11619840 0.00091564
Fe 5.50179503 6.26878574 1.23254728
Fe 1.33445424 0.93289141 5.64593162
Fe 1.51505720 2.90463316 6.92021589
Fe 1.48289389 4.09400476 -0.06697406
Fe 1.45541860 6.27232640 1.20197879
Fe 6.69064194 5.97847797 3.36425368
Fe 6.67804899 4.80982176 5.54296575
Fe 0.15102514 5.96018465 3.30782314
Fe 0.43471329 4.69553491 5.58369669
Fe 6.73357644 2.46565611 1.36489589
Fe 6.76074652 1.27664779 3.47500035
Fe 0.20120731 2.43151043 1.34792391
Fe 0.16600241 1.25788353 3.49982428
S 2.12654434 5.54552891 7.07549504
Fe 4.78123901 5.29797052 6.85842810
Fe 2.15704512 -0.24238657 3.60724505
Fe 4.61554923 -0.27702375 3.51598855
Fe 2.22106838 7.46070248 3.25817228
Fe 4.62056032 7.40292052 3.32281229
Fe 2.21250750 1.73026804 0.06921410
Fe 4.73872869 1.71225114 0.10852046

$Fe_{49}S_6$

Fe 3.45694611 3.55745031 3.57825170
Fe 5.39544286 4.15551371 2.53013901
Fe 5.43748852 2.94405673 4.65148208
Fe 1.51968522 4.15552337 2.52896071
Fe 1.47598504 2.94474128 4.65179717
Fe 2.23141696 5.27552861 4.58178556
Fe 4.68138435 5.27572927 4.58161252
Fe 2.25891288 1.87899345 2.59642049
Fe 4.65505066 1.87780964 2.59719405
Fe 3.45607148 1.50691833 4.69168715
Fe 3.45701027 3.63223928 6.01077925
Fe 3.45900142 3.48840978 1.30484769
Fe 3.45744279 5.56243747 2.48644278
Fe 7.44355315 4.78410146 1.29631273
Fe 7.49793474 3.57271445 3.43246357
Fe 7.78663614 2.19879073 5.27471305
Fe -0.52701476 4.78421517 1.29297560
Fe -0.58383484 3.57380830 3.42932817
Fe -0.87755191 2.20175474 5.27201808
Fe 0.77605327 7.29391369 5.11445867
Fe 3.45485278 7.11023911 5.41284733
Fe 6.13675119 7.29272368 5.11715869
Fe 0.98938055 0.10174309 1.43835056
Fe 3.45538951 0.07393295 1.48530399
Fe 5.92023756 0.09975246 1.43764639

Fe 3.45261970 -0.94788264 5.36503886
S 3.45146757 0.70564683 6.82113370
S 3.45006725 3.68309317 8.12279519
Fe 3.46162193 3.41111974 -1.14774557
Fe 3.45944148 5.54987509 0.04563894
Fe 3.45919037 7.67787100 1.20577261
Fe 5.50787664 0.78555862 5.60171172
S 6.25830142 2.72997362 6.76842045
Fe 5.45713991 4.09973407 0.09256746
Fe 5.46640303 6.25371090 1.30052827
Fe 1.40011756 0.78709299 5.60116806
S 0.64936360 2.72906684 6.76799097
Fe 1.46360994 4.09967452 0.09138725
Fe 1.44978015 6.25379320 1.29795896
Fe 6.73825193 5.90903132 3.36066223
Fe 6.77456835 4.69282983 5.49130257
Fe 0.17583160 5.90950809 3.35854122
Fe 0.13555002 4.69291467 5.48821612
Fe 6.70849604 2.43473268 1.41734793
Fe 6.71415738 1.16004268 3.50456071
Fe 0.20594977 2.43602768 1.41420172
Fe 0.19757418 1.16315065 3.50324381
S 1.71805099 6.04709751 6.66773348
S 5.18768299 6.04731044 6.66880967
Fe 2.18590171 -0.28189886 3.54503148
Fe 4.72272937 -0.28433628 3.54523670
Fe 2.22758193 7.40079171 3.31241700
Fe 4.68678680 7.40122932 3.31463910
Fe 2.22354652 1.75345850 0.16254611
Fe 4.69257090 1.75283287 0.16277285

Fe_{55} with nanocap(10,0)

Fe 9.78536003 10.20204340 7.77851012
Fe 11.87623676 10.17444319 8.79676268
Fe 9.77226284 10.25274716 10.10552450
Fe 9.77640719 10.17103825 5.47264411
Fe 7.74298864 10.22397581 6.75260158
Fe 9.20536112 12.16574926 6.74357142
Fe 10.47490376 12.20166934 8.80867651
Fe 9.12101483 8.24267334 6.80867658
Fe 10.40118356 8.22303966 8.85586571
Fe 8.09024201 9.01825336 8.84019462
Fe 8.12603729 11.49066189 8.77987857
Fe 11.41260082 8.93923727 6.76734868
Fe 11.47113451 11.37486022 6.73829752
Fe 14.08774436 10.11272318 9.52769407
Fe 12.08376409 10.33431886 11.18495353
Fe 9.87562165 10.27524670 12.42191520
Fe 9.77743364 10.12998584 3.12605277
Fe 7.65380195 10.19354707 4.36608828
Fe 5.59776384 10.25141859 5.53151280
Fe 8.62598481 14.28421821 5.61425888
Fe 9.87648084 14.24007838 7.71580701
Fe 11.21862689 14.18604252 9.81063310

Fe 8.41655634 6.11273838 5.73763276
Fe 9.68750523 6.15478767 7.83646690
Fe 10.91939025 6.22581836 9.99286968
Fe 6.30264805 7.81173867 9.81331870
Fe 6.30244920 10.32201519 9.56956998
Fe 6.40896112 12.83751206 9.69202878
Fe 13.04552549 7.51571270 5.58915435
Fe 13.18208086 10.09593849 5.57496022
Fe 13.16289854 12.67068240 5.51675580
Fe 8.09675110 8.89052402 11.26099513
Fe 7.90804456 11.44353177 11.16539111
Fe 13.59005079 8.83927787 7.59578652
Fe 13.64638350 11.39732801 7.56548614
Fe 5.94133899 8.99020426 7.66313465
Fe 5.99472696 11.54680058 7.59551429
Fe 11.45031580 8.84654304 4.39716144
Fe 11.50812183 11.37559304 4.35208288
Fe 12.65053380 12.19264705 9.70421382
Fe 10.38335954 12.31000408 11.20990616
Fe 9.17283125 12.20218499 4.36245652
Fe 7.09783357 12.26851354 5.59127598
Fe 12.56878933 8.13203589 9.76322029
Fe 10.66621081 8.32622108 11.20240832
Fe 9.08094634 8.13094744 4.42279638
Fe 7.01472365 8.18341035 5.66310659
Fe 7.51268633 13.53546730 7.66868660
Fe 8.80052178 13.51785974 9.79372272
Fe 7.38571055 6.95879417 7.77593485
Fe 8.62940718 6.95458479 9.98056050
Fe 10.88887689 13.46891708 5.57951996
Fe 12.19191949 13.45272975 7.66074593
Fe 10.72421949 6.83810497 5.68735222
Fe 12.04290897 6.87326079 7.75499866
C 8.79619664 13.86873940 11.71953133
C 11.26732747 14.00274706 11.78225545
C 9.99493315 14.17648083 12.48368161
C 6.54817156 12.85310985 11.63726319
C 7.62283088 13.38486430 12.45212656
C 5.75397891 10.51387732 11.36861195
C 5.95301360 11.67731683 12.21198182
C 6.27809902 8.09896555 11.75967205
C 5.84365714 9.36114967 12.26422141
C 8.30316813 6.76723934 11.92296158
C 7.20765451 7.40448346 12.63489004
C 10.77178952 6.49144035 11.95676522
C 9.50782543 6.44469825 12.68067428
C 12.76809750 7.87974605 11.70354360
C 11.88329615 7.17313131 12.61460109
C 14.06409796 10.04761188 11.44901477
C 13.54002582 8.95908068 12.27154155
C 13.05235649 12.33027706 11.61199883
C 13.73969755 11.24165177 12.24190360
C 12.24350381 13.17838624 12.48496272
C 6.82626786 9.04397951 14.53905629
C 7.48128475 9.76652661 15.62211777

C 6.08831530 9.81873490 13.60747144
C 6.17377276 11.24064526 13.57722273
C 7.57018007 11.23200912 15.58255832
C 7.00290338 11.96572452 14.45933405
C 8.86001949 7.75065924 15.95851692
C 8.38147353 7.15044363 14.76982999
C 7.33228981 7.76822487 14.05382677
C 8.47763059 9.05290270 16.36316439
C 10.83755249 8.92025461 16.36454791
C 11.89473647 9.52671479 15.61896696
C 9.69970539 9.72067812 16.78786362
C 11.98150524 10.98960198 15.58607355
C 9.78013867 11.09030899 16.75421198
C 11.00020481 11.74011240 16.30113790
C 13.27672316 9.42500781 13.61366764
C 13.38338082 10.85167128 13.59797887
C 10.71657850 7.00528933 14.77002715
C 9.51054140 6.55890014 14.07362948
C 10.31358812 7.66564152 15.95552927
C 11.80809723 7.52882251 14.03672486
C 12.44473969 8.74156263 14.52303296
C 12.63506436 11.66273107 14.46827492
C 12.14856795 12.92519686 13.92010908
C 8.64179239 11.86743958 16.28770584
C 11.10388814 13.58320797 14.62263253
C 9.96301184 14.10180498 13.89016842
C 10.62060335 13.02689541 15.83378430
C 9.16951727 13.09810915 15.82460651
C 8.77219435 13.67408350 14.59085570
C 7.67067987 13.13704555 13.89469175

Fe_{55} with nanocap(6,6)

Fe 9.86469974 10.06873770 13.07014607
Fe 11.95732198 10.10286104 14.07708863
Fe 9.85611965 10.10710996 15.38490949
Fe 9.90789078 9.99903454 10.77736193
Fe 7.85327486 10.00113966 12.01131118
Fe 9.23983924 11.96292855 11.97958137
Fe 10.46224807 12.06175070 14.09096193
Fe 9.26634392 8.07849589 12.10917692
Fe 10.54096711 8.11253853 14.12657526
Fe 8.20167713 8.85847577 14.12550332
Fe 8.15440411 11.29285870 14.06225276
Fe 11.54489802 8.85723282 12.06058192
Fe 11.51898349 11.27803684 12.05362192
Fe 14.18191148 10.03499338 15.05992557
Fe 12.08526231 10.15055514 16.47011117
Fe 9.92749751 10.05093903 17.84872792
Fe 9.95616071 9.93391903 8.32573635
Fe 7.81237819 9.93238430 9.57188003
Fe 5.72344291 9.86814394 10.74219662
Fe 8.64083581 13.99709422 10.68644132
Fe 9.80229268 14.07935208 12.92404910
Fe 11.15428133 14.14193211 15.02682540

Fe 8.62581812 5.95639487 11.09680537
Fe 9.95440111 5.99667112 13.14049856
Fe 11.35535148 6.09274790 15.20516251
Fe 6.48473781 7.52203681 15.11400758
Fe 6.30729534 10.09957982 15.01920871
Fe 6.11369834 12.76325687 14.47182466
Fe 13.29093729 7.56933718 10.88601321
Fe 13.25604990 10.10796195 10.86375630
Fe 13.28154777 12.57546717 10.97322127
Fe 8.15098972 8.80740680 16.54786277
Fe 8.11939135 11.28499153 16.59016871
Fe 13.78210298 8.87801754 12.85267030
Fe 13.72933620 11.33202699 13.00654692
Fe 6.06313536 8.76920363 12.99298164
Fe 6.03151522 11.20268294 12.78269956
Fe 11.61471806 8.76741275 9.61692199
Fe 11.56874828 11.29079300 9.62360948
Fe 12.63997945 12.21438551 14.99604044
Fe 10.45826296 12.15697061 16.53500331
Fe 9.25128933 11.97164999 9.54065636
Fe 7.13911754 11.95915999 10.76751212
Fe 12.78157080 8.03540379 14.80831198
Fe 10.68863564 8.12628680 16.55111760
Fe 9.23459538 7.97738844 9.68132335
Fe 7.13773363 7.92387026 10.95549812
Fe 7.52273996 13.29931937 12.75060504
Fe 8.66747479 13.44937336 15.01027420
Fe 7.54252941 6.75194862 13.10144108
Fe 8.81812616 6.78892715 15.16699381
Fe 10.93688234 13.31622333 10.86785740
Fe 12.20053682 13.37229177 12.99082443
Fe 10.91950966 6.78214857 10.93139015
Fe 12.26180192 6.76325130 12.92894471
C 10.23112954 6.07347732 16.85142909
C 8.83631314 6.24756231 16.98059559
C 12.75089903 7.36639042 16.62743794
C 12.39581593 6.80077653 17.90166338
C 11.07278866 6.18350150 18.04012110
C 13.59659248 8.54376507 16.55281895
C 13.93388741 11.33230529 16.56596117
C 14.12349029 9.14327543 17.75725778
C 14.31141849 10.59824735 17.77467770
C 13.31683895 12.59234814 16.69708627
C 11.00714911 14.18818148 16.91647253
C 13.00645914 13.16174901 17.96754209
C 11.67107540 13.73976118 18.09622005
C 9.60228185 14.10027694 16.77404268
C 7.10410564 13.00752705 16.20075059
C 8.85093964 13.61455731 17.91517776
C 7.55961220 13.11101920 17.57692088
C 6.17740072 11.77947402 16.18272909
C 5.93135178 9.00049069 16.75750168
C 5.90555691 9.92282808 17.88071047
C 6.13249519 11.29697827 17.54594039
C 6.40226100 7.68828529 17.00036441

C 6.99758497 7.30661798 18.25548370
C 8.18831505 6.45966456 18.24429959
C 7.98016552 9.56425207 20.83126133
C 7.74048172 8.19558552 20.45269575
C 6.32266641 9.51110967 19.16649531
C 6.79160218 8.16568925 19.37264841
C 7.10739624 10.37637312 20.04016010
C 10.03902029 7.68344254 21.08549128
C 8.78255491 7.28542111 20.51536349
C 10.31120500 9.03420606 21.47687614
C 9.25719307 10.02312043 21.24903171
C 13.81278300 9.19151262 20.21781952
C 14.04753139 10.57139713 20.23812825
C 12.72074412 8.61810464 20.97637203
C 11.70058907 9.46462393 21.53777667
C 11.97220986 10.86647898 21.55451444
C 13.21230359 11.38494546 21.05977067
C 13.92686924 8.45337937 18.98297309
C 14.31119353 11.29361350 19.00402123
C 11.04898452 6.91460901 20.40773727
C 10.43403069 6.21104825 19.30522661
C 9.00837106 6.38942688 19.39726065
C 13.04903458 7.31687175 19.05145262
C 12.34551503 7.40429903 20.30703752
C 9.61843318 11.40776739 20.93947359
C 10.94399588 11.81116455 21.18602014
C 7.55538745 11.64277606 19.60056261
C 6.96970772 12.10252040 18.38617987
C 13.62498487 12.57705033 19.09495278
C 8.82406044 12.19166353 20.00733556
C 10.88742307 13.42234563 19.28920063
C 12.95976593 12.61218475 20.35880579
C 11.55839862 12.86143326 20.39989443
C 9.46620778 13.19576839 19.15810801

$Fe_{54}S$ with nanocap(10,0)

Fe 9.78680412 10.20189079 7.78038966
Fe 11.89380677 10.14674373 8.79486804
Fe 9.77530860 10.24902935 10.07324320
Fe 9.77329878 10.15561499 5.47395279
Fe 7.73859605 10.24818729 6.76390601
Fe 9.22350563 12.16213791 6.75330416
Fe 10.50622736 12.16550941 8.83204001
Fe 9.09307565 8.24188223 6.83504125
Fe 10.36839875 8.23600909 8.91205825
Fe 8.06034266 9.04752842 8.85251616
Fe 8.14513736 11.51709124 8.79975876
Fe 11.38005464 8.90828075 6.78630082
Fe 11.46349508 11.34550472 6.73890291
Fe 14.12896053 10.07855001 9.55169107
Fe 12.09450502 10.19245138 11.19215089
S 9.71829800 10.28493683 12.30789730
Fe 9.76796392 10.10890636 3.13159155
Fe 7.64373441 10.20005972 4.36962163

Fe 5.59054536 10.28635712 5.55305452
Fe 8.66938579 14.27521057 5.61037455
Fe 9.93546688 14.21041147 7.73375837
Fe 11.26405719 14.18647880 9.82215924
Fe 8.39526343 6.12299415 5.79087859
Fe 9.66665948 6.19005213 7.90401497
Fe 10.96477496 6.20653203 9.99197908
Fe 6.24078001 7.86237325 9.80025617
Fe 6.30898685 10.36492045 9.56759828
Fe 6.42410742 12.87681520 9.69295503
Fe 13.02051630 7.49538146 5.60305431
Fe 13.14495251 10.04928514 5.61244962
Fe 13.19134370 12.60484639 5.50637232
Fe 7.90230349 9.06519376 11.26436801
Fe 7.99037534 11.60038552 11.20950913
Fe 13.54541136 8.79171415 7.63959583
Fe 13.63153550 11.34876517 7.59059890
Fe 5.92550816 9.03944213 7.65785026
Fe 6.01409132 11.61100795 7.59883645
Fe 11.44566450 8.81683296 4.38505757
Fe 11.52682358 11.34248041 4.33490441
Fe 12.67722445 12.15982003 9.69383186
Fe 10.56252353 12.23791439 11.25644193
Fe 9.20227184 12.19382458 4.35604568
Fe 7.13499924 12.28193028 5.59376237
Fe 12.52967933 8.11311231 9.77407975
Fe 10.44582979 8.26037486 11.32853527
Fe 9.07228632 8.11342945 4.44213013
Fe 7.00284751 8.20895698 5.68156119
Fe 7.56280560 13.56301595 7.67563908
Fe 8.83558862 13.52150982 9.79210555
Fe 7.34343384 6.99699916 7.81890737
Fe 8.59771628 7.04393433 9.93436322
Fe 10.92525810 13.42375284 5.59504688
Fe 12.22648036 13.39195285 7.67256459
Fe 10.70564556 6.82352417 5.72562791
Fe 12.00129704 6.85487005 7.79788221
C 8.72085205 13.84715417 11.71830445
C 11.22211331 14.03554839 11.77602936
C 9.93712515 14.14395310 12.47106692
C 6.47462586 12.83863298 11.64068841
C 7.54723097 13.38729187 12.46025591
C 5.74510527 10.45240978 11.35993704
C 5.94675728 11.62417205 12.20386718
C 6.25681329 8.02351312 11.74446066
C 5.84462255 9.30353887 12.25395449
C 8.40006957 6.82360539 11.87153346
C 7.27279476 7.41241902 12.59123069
C 10.87309703 6.42177876 11.94059443
C 9.58695447 6.45421073 12.63912737
C 12.81191022 7.91443571 11.69975344
C 11.93548324 7.18663386 12.60726088
C 14.08450579 10.08227623 11.45476063
C 13.58300007 8.97809452 12.27908959
C 13.01952984 12.36402594 11.60625289

C 13.69708279 11.26416604 12.23268794
C 12.20684027 13.20248428 12.47851815
C 6.84143591 9.00772040 14.52653931
C 7.48156158 9.73199877 15.61396540
C 6.09776586 9.77366354 13.59768199
C 6.16167690 11.19116229 13.56725412
C 7.54881990 11.19928728 15.58037408
C 6.97363090 11.92828646 14.46169896
C 8.88940755 7.73283063 15.93565327
C 8.42993834 7.14671667 14.73001002
C 7.37489653 7.75028618 14.01868938
C 8.48941983 9.02624995 16.34651110
C 10.85126905 8.91940459 16.35729663
C 11.90449024 9.53693703 15.61770352
C 9.70354265 9.70647336 16.77608814
C 11.97149803 11.00003141 15.58654989
C 9.76610250 11.07707375 16.74533503
C 10.97965431 11.74044707 16.29724669
C 13.29624066 9.45018560 13.62133023
C 13.36532497 10.87586910 13.59314939
C 10.76195639 7.00523758 14.75850980
C 9.56866213 6.58001410 14.03905896
C 10.34234830 7.66059011 15.94080327
C 11.85767472 7.53272261 14.02979084
C 12.47107063 8.75653007 14.52422746
C 12.60684287 11.67851184 14.46279667
C 12.10431750 12.92979829 13.91503119
C 8.61740651 11.84385651 16.28363338
C 11.05971579 13.58087861 14.61767200
C 9.90925515 14.07374807 13.87592246
C 10.58487162 13.02169583 15.82838996
C 9.13139227 13.07820494 15.82104439
C 8.72575953 13.64616781 14.58759919
C 7.61938890 13.10848272 13.90070891

$Fe_{54}S$ with nanocap(6,6)

Fe 9.86404887 10.05767947 13.01554352
Fe 11.94729179 10.08362663 14.05541585
Fe 9.86290350 10.09119181 15.32123871
Fe 9.89923046 10.00830679 10.73981071
Fe 7.84738192 10.00738164 11.98329162
Fe 9.23610220 11.96038061 11.95839160
Fe 10.47016178 12.04722723 14.06345537
Fe 9.26147382 8.07894151 12.06056122
Fe 10.52853227 8.10805444 14.09288452
Fe 8.20031985 8.85286724 14.08913125
Fe 8.15845478 11.28623305 14.06786629
Fe 11.53534477 8.85422179 12.01975239
Fe 11.51990834 11.26836664 12.02175931
Fe 14.17566848 10.01320680 15.06366134
Fe 12.12740626 10.12039216 16.42448524
S 9.94963618 10.02832033 17.55523050
Fe 9.94961609 9.94601826 8.29984225
Fe 7.80042699 9.95034131 9.54336604

Fe 5.71738138 9.87529183 10.73044935
Fe 8.63581385 14.00017107 10.68130962
Fe 9.81332043 14.06351136 12.93243477
Fe 11.18066715 14.12579600 15.03417800
Fe 8.62060330 5.96061409 11.02983091
Fe 9.92771283 5.99686481 13.09576285
Fe 11.28759109 6.06054683 15.17666269
Fe 6.48126562 7.50599856 15.11428987
Fe 6.31726693 10.10021896 15.04240104
Fe 6.12793295 12.74710576 14.48850620
Fe 13.29139044 7.56391955 10.87855659
Fe 13.26586696 10.09480451 10.84936633
Fe 13.29078934 12.56082068 10.95255908
Fe 8.11157838 8.79689081 16.49771122
Fe 8.12466827 11.28050340 16.61823439
Fe 13.75460034 8.85914050 12.86321762
Fe 13.72662118 11.31556192 12.99491387
Fe 6.06606336 8.76789112 12.98242062
Fe 6.02428136 11.20508013 12.77794912
Fe 11.61309665 8.77156714 9.59750185
Fe 11.57286428 11.29480192 9.59927993
Fe 12.64040294 12.19499496 14.98681819
Fe 10.45826113 12.18114076 16.49050224
Fe 9.24547989 11.98582293 9.51731241
Fe 7.13288756 11.97055820 10.75748578
Fe 12.75496031 7.99528899 14.85231093
Fe 10.69143301 8.05007885 16.49440149
Fe 9.22817294 7.98450816 9.64287043
Fe 7.13212356 7.93638932 10.91959522
Fe 7.52477149 13.30301547 12.75415489
Fe 8.67195061 13.42283412 15.04776387
Fe 7.53284542 6.75409382 13.04691368
Fe 8.79357335 6.78809426 15.14279237
Fe 10.93113338 13.30922869 10.85772870
Fe 12.21167206 13.36740390 12.96122317
Fe 10.91945437 6.77654336 10.89924759
Fe 12.24210660 6.76624423 12.92316664
C 10.28119287 6.04330890 16.88297971
C 8.88871892 6.27201036 16.97838498
C 12.77848772 7.37129612 16.67396443
C 12.42893401 6.78673353 17.94029045
C 11.11038872 6.15883792 18.07715980
C 13.62268286 8.53728131 16.58894848
C 13.93340782 11.30345404 16.58976556
C 14.15301093 9.13782066 17.79484091
C 14.33076929 10.59413905 17.80640324
C 13.27552987 12.54567271 16.71310595
C 10.97228609 14.17312850 16.93097461
C 12.96841538 13.13152601 17.97754046
C 11.63528734 13.71635970 18.11058005
C 9.56587120 14.08423160 16.80959724
C 7.09882990 12.99400636 16.23947478
C 8.81762279 13.62217486 17.96538975
C 7.53292658 13.11577714 17.62574163
C 6.18289806 11.77063885 16.21923419

C 5.93383201 9.01511438 16.77934319
C 5.89510720 9.92643654 17.91411512
C 6.11368178 11.30057361 17.59063221
C 6.41013224 7.70049173 17.00790249
C 7.02645498 7.32363656 18.25655885
C 8.22556402 6.48553501 18.23923225
C 7.97881095 9.56163916 20.86196777
C 7.74777832 8.19588291 20.46900788
C 6.32290564 9.50700070 19.19377229
C 6.80417142 8.16445504 19.38624760
C 7.10284673 10.37251907 20.07214075
C 10.04314956 7.69180326 21.10316924
C 8.79447017 7.29223605 20.52416491
C 10.30637110 9.04070274 21.50660539
C 9.24796653 10.02721871 21.29120638
C 13.81528779 9.20109670 20.25492513
C 14.04346100 10.58102998 20.26830601
C 12.71975576 8.62856259 21.00886778
C 11.69472213 9.47281557 21.56714584
C 11.96169196 10.87533815 21.58240704
C 13.19822868 11.39360157 21.08107732
C 13.94124583 8.45813883 19.02253723
C 14.30786372 11.29579142 19.02985977
C 11.05863631 6.92066658 20.43530489
C 10.45674510 6.20859159 19.33158270
C 9.03120528 6.40413160 19.40099442
C 13.06604820 7.31834778 19.09068823
C 12.35373513 7.41059625 20.34222028
C 9.60042691 11.41353487 20.98116537
C 10.92757119 11.81807155 21.21717601
C 7.52990670 11.65203997 19.65055620
C 6.93730293 12.11306637 18.43819357
C 13.59925182 12.56957252 19.10914103
C 8.79959404 12.19948174 20.05478930
C 10.85995152 13.42052448 19.31548719
C 12.93984619 12.61571677 20.37398359
C 11.53766541 12.86452724 20.42323296
C 9.43631624 13.20419633 19.20433454

$Fe_{52}S_3$ with nanocap(10,0)

Fe 9.75518349 10.23213980 7.82996535
Fe 11.94934242 10.14692948 8.82320712
Fe 9.43540053 10.43282002 10.23163102
Fe 9.76945769 10.19961447 5.57441302
Fe 7.71411179 10.27644788 6.81425270
Fe 9.22040052 12.18972353 6.80462620
Fe 10.45985364 12.20523954 8.91011362
Fe 9.07802343 8.28650526 6.83828333
Fe 10.37447044 8.23430508 8.85255292
Fe 8.01889791 9.00844473 8.84513732
Fe 8.06844309 11.61872200 8.77883636
Fe 11.37292608 8.95663326 6.80902242
Fe 11.45451927 11.38540494 6.81143728
Fe 14.15376884 10.08119845 9.61488976

S 11.50535116 10.80031212 10.84489422
Fe 11.43202838 9.16667897 12.39913734
Fe 9.79187265 10.16755692 3.11168897
Fe 7.69502783 10.22712962 4.35552005
Fe 5.60129033 10.27147338 5.56604443
Fe 8.69286409 14.28795537 5.61123718
Fe 9.92361744 14.24189088 7.74418974
Fe 11.27052303 14.16948285 9.85772526
Fe 8.40871612 6.15692362 5.81500034
Fe 9.63771833 6.19023375 7.94422264
Fe 10.92062902 6.22952483 10.09581135
Fe 6.20559251 7.79743647 9.80602611
Fe 6.23458021 10.37731204 9.44729592
Fe 6.42609060 12.85336468 9.64553152
Fe 13.00081431 7.52967672 5.67245031
Fe 13.15848817 10.08796070 5.67746301
Fe 13.21402695 12.64296778 5.63708276
Fe 7.71376391 9.21082630 11.26568076
S 9.29029521 10.59879257 12.56321551
Fe 13.57984578 8.78893512 7.66466615
Fe 13.67055375 11.36496717 7.64707722
Fe 5.86028188 8.98692815 7.61656314
Fe 5.84572643 11.67474048 7.51222691
Fe 11.43016604 8.87182816 4.37549901
Fe 11.52407080 11.37813931 4.37592849
Fe 12.81535804 12.22430173 9.79588067
Fe 10.02009795 12.43263026 11.32421621
Fe 9.22425176 12.21301444 4.37558952
Fe 7.13920493 12.29352689 5.61255165
Fe 12.54808037 8.10509572 9.79868788
S 9.93238496 8.42324084 10.92223781
Fe 9.08475052 8.16949938 4.42889380
Fe 6.99486750 8.20863611 5.67064256
Fe 7.48013956 13.68887613 7.60821000
Fe 8.76103454 13.65236207 9.75146304
Fe 7.31360108 6.95651997 7.82326411
Fe 8.52289911 6.97943002 10.05082631
Fe 10.95638235 13.47114020 5.65785946
Fe 12.23148624 13.42387927 7.75778295
Fe 10.70440787 6.85430073 5.77077328
Fe 11.98574869 6.83821364 7.84073661
C 8.75827241 14.00891553 11.69304491
C 11.28455819 13.96022294 11.79093895
C 9.99666112 14.23444962 12.45777733
C 6.66055572 12.73820802 11.55357748
C 7.60087245 13.42834543 12.39315029
C 5.78517838 10.38011200 11.28033937
C 6.05152853 11.58070072 12.08707247
C 6.24231732 7.94165294 11.75724727
C 5.81528139 9.25009078 12.21597043
C 8.29916949 6.54710033 11.96964236
C 7.22777503 7.29279831 12.63331456
C 10.83914304 6.30675146 12.01320162
C 9.54144682 6.30212132 12.70644252
C 12.86581998 7.83358617 11.72103591

C 11.92547657 7.12912515 12.61655536
C 14.13712048 10.12872916 11.48267555
C 13.55894498 9.00347157 12.24919011
C 13.29862503 12.51587487 11.71505323
C 13.85761488 11.33539041 12.29046469
C 12.36089603 13.26941323 12.52472499
C 6.82855122 9.01108437 14.49168647
C 7.47024685 9.76872978 15.56101153
C 6.11384470 9.76718154 13.54078529
C 6.22330463 11.19160298 13.45921834
C 7.54670243 11.23501837 15.50529166
C 7.00491260 11.95190158 14.35847551
C 8.85275881 7.76928817 15.94828740
C 8.38224433 7.12424439 14.77535452
C 7.33323919 7.70745353 14.03860792
C 8.45658284 9.07396882 16.32796172
C 10.81127289 8.97499390 16.34439857
C 11.85341298 9.59484254 15.59894472
C 9.66597677 9.76106626 16.76306853
C 11.96200749 11.05194217 15.57851873
C 9.73536901 11.12845137 16.71821985
C 10.95853725 11.78709548 16.27836385
C 13.22599508 9.50720143 13.57390183
C 13.40380124 10.93325516 13.59654978
C 10.70684406 7.02970438 14.77766087
C 9.52539295 6.54473538 14.09268995
C 10.30188056 7.70917575 15.94667794
C 11.78140919 7.56352844 14.01367153
C 12.37264972 8.82569035 14.47585913
C 12.64865990 11.73305796 14.48451141
C 12.17815993 13.00025055 13.94455202
C 8.59699069 11.88787299 16.22797332
C 11.08329007 13.62498452 14.61014208
C 9.94693355 14.12280305 13.86433783
C 10.57592203 13.06623086 15.80724052
C 9.12012903 13.12192632 15.77093649
C 8.73693791 13.70131295 14.54130598
C 7.64352473 13.15446570 13.81848391

$Fe_{52}S_3$ with nanocap(6,6)

Fe 9.90763813 10.04024731 13.06229474
Fe 12.03021620 10.02242909 14.14448233
Fe 9.77494891 10.18769703 15.41422370
Fe 9.95673773 9.98760505 10.79418489
Fe 7.90253240 9.99340899 12.00114398
Fe 9.28901776 11.93863745 11.98938054
Fe 10.52004928 12.06746881 14.07053055
Fe 9.32466282 8.06423568 12.08014648
Fe 10.60178063 8.03567304 14.14321860
Fe 8.21344386 8.80047351 14.09297157
Fe 8.14682284 11.28544998 14.03774950
Fe 11.61254697 8.81023219 12.08504962
Fe 11.57708090 11.22316510 12.06571208
Fe 14.24193305 10.07952818 15.03180093

S 11.76422606 10.55298869 16.28853559
Fe 10.65568248 9.51740493 17.94698834
Fe 10.02019483 9.93429441 8.33661592
Fe 7.85995833 9.94751812 9.56334024
Fe 5.76650143 9.86349117 10.75114355
Fe 8.71269328 14.00322372 10.72885676
Fe 9.83751632 14.05983627 13.01253348
Fe 11.25775991 14.14266089 15.03163464
Fe 8.65337913 5.94873229 11.02161588
Fe 9.96555685 5.95899150 13.10060335
Fe 11.30734176 6.02392095 15.18895455
Fe 6.52320111 7.42029299 15.10685649
Fe 6.29367132 10.17968109 15.11025896
Fe 6.27691192 12.65970303 14.55789806
Fe 13.32439932 7.50991756 10.88816537
Fe 13.31562390 10.06081739 10.83501183
Fe 13.34144092 12.52180054 10.94069330
Fe 7.93559192 8.93654323 16.38795205
S 8.89142467 10.74937346 17.40634032
Fe 13.89882131 8.82389886 12.81947031
Fe 13.78216721 11.28754247 12.98002927
Fe 6.09732031 8.78226376 13.03621109
Fe 6.00264066 11.22597699 12.72969891
Fe 11.65266072 8.73811849 9.62635187
Fe 11.61423916 11.27767026 9.64156036
Fe 12.74435379 12.19982823 15.07604863
Fe 10.37314848 12.30145502 16.41086035
Fe 9.30083910 11.97634280 9.55327924
Fe 7.20196754 11.95736319 10.77425682
Fe 12.90898134 7.93563359 14.75633657
S 10.04683199 8.20168491 16.25044768
Fe 9.26181110 7.98016629 9.67009738
Fe 7.16838723 7.93537922 10.96347410
Fe 7.52547480 13.34804940 12.72000060
Fe 8.60968173 13.40739718 15.13993795
Fe 7.58960792 6.68750387 13.04664694
Fe 8.80364658 6.62002143 15.28290618
Fe 10.98058293 13.28893315 10.93019816
Fe 12.32656955 13.36327507 12.96037635
Fe 10.95239251 6.73195189 10.90006856
Fe 12.32771472 6.64372220 12.89631754
C 10.14801645 5.70460995 16.87113694
C 8.76076627 5.86255553 17.03643776
C 12.93420240 7.24625000 16.55037394
C 12.38532475 6.74560520 17.79012329
C 11.06223705 6.06758741 17.96316870
C 13.76220172 8.39363879 16.46840413
C 14.19098842 11.55008325 16.51774096
C 14.16498891 9.16970780 17.62810475
C 14.36795729 10.65393077 17.66844964
C 13.51352366 12.76764664 16.69566602
C 10.85165365 14.20517727 16.91461782
C 12.96823215 13.21897465 17.92761832
C 11.57730074 13.71671692 18.05519083
C 9.43359061 14.07471465 16.86922338

C 6.99352590 13.04617453 16.35947166
C 8.65802803 13.70174101 18.05222358
C 7.35398453 13.25503634 17.75615264
C 6.11839064 11.86715016 16.33498464
C 5.91219378 9.11913238 16.81772638
C 5.82160230 10.02860305 17.96142792
C 5.94407943 11.41967550 17.70107056
C 6.37290025 7.77387526 16.98147361
C 7.00258015 7.32722084 18.21050473
C 8.13651614 6.37041111 18.22525111
C 7.96783551 9.56908984 20.82936854
C 7.74776542 8.20821798 20.41213867
C 6.30032011 9.54397594 19.19943364
C 6.81019479 8.19444536 19.32984845
C 7.06364232 10.39879200 20.08923578
C 10.04096168 7.69082912 21.01987040
C 8.78717348 7.29642406 20.45536815
C 10.30146450 9.03406376 21.42743074
C 9.23562388 10.02570278 21.24954972
C 13.77083047 9.21770180 20.11052506
C 14.00780258 10.58865959 20.15326641
C 12.70005814 8.63249889 20.88496750
C 11.68876989 9.46562808 21.47745380
C 11.94787112 10.86722953 21.50670421
C 13.17380868 11.38782568 20.99747725
C 13.86511676 8.51145953 18.85264152
C 14.26569779 11.31385187 18.92408982
C 11.04261012 6.92166990 20.32349503
C 10.42850287 6.20100586 19.23025561
C 8.99690625 6.38569704 19.35211124
C 12.98619779 7.36078900 18.92309041
C 12.32333021 7.42676129 20.20494003
C 9.56566549 11.41764881 20.95485700
C 10.90205446 11.80955211 21.15746794
C 7.40997793 11.73070807 19.72078237
C 6.73613268 12.25392807 18.56983399
C 13.56591109 12.59606418 19.05047453
C 8.72343953 12.23901950 20.08882402
C 10.80224217 13.41132221 19.27080653
C 12.90585832 12.61446374 20.30641759
C 11.50214323 12.85908728 20.36452956
C 9.35378714 13.24443801 19.23625954

$Fe_{49}S_6$ with nanocap(10,0)

Fe 9.78045069 10.19539069 7.62426578
Fe 11.90309530 10.12290150 8.55141915
Fe 9.73852791 10.26427082 9.97698346
Fe 9.72647054 10.13320037 5.31045024
Fe 7.71332376 10.27377760 6.59659083
Fe 9.21735485 12.16839205 6.53218249
Fe 10.52585809 12.18762092 8.58401937
Fe 9.06246783 8.25248725 6.63289360
Fe 10.35139182 8.19599421 8.67998350
Fe 8.04030117 9.03265366 8.61324359

Fe 8.15444005 11.54598875 8.57753886
Fe 11.37172148 8.87264170 6.56055725
Fe 11.46521199 11.32883223 6.51370440
Fe 14.26331096 10.05328461 9.59422965
S 12.30989814 10.09075422 10.64104417
S 10.18142597 9.75145441 12.26200168
Fe 9.74856227 10.12500759 2.96930002
Fe 7.56471689 10.22219944 4.26002484
Fe 5.54264671 10.40022955 5.52065007
Fe 8.70362669 14.19019496 5.50985517
Fe 9.93955599 14.23761774 7.67195809
Fe 11.23670435 14.18838383 9.90615188
Fe 8.29782858 6.17211492 5.65143797
Fe 9.59641692 6.18527055 7.83142135
Fe 11.07912963 5.91002768 9.89984644
Fe 6.22845911 7.77139344 9.92620733
Fe 6.32233530 10.37501181 9.76191796
Fe 6.38829157 12.91175753 9.78938537
Fe 13.00745292 7.57095716 5.60004541
Fe 13.21834612 10.02824273 5.56247901
Fe 13.24970469 12.48960281 5.49524775
S 7.90001848 9.00737373 10.74196523
S 7.95647869 11.60831907 10.70884061
Fe 13.57049506 8.73872767 7.69156498
Fe 13.61982818 11.36343186 7.63446097
Fe 5.91497470 9.09711322 7.68577295
Fe 6.01304207 11.60963726 7.62638020
Fe 11.36735291 8.90343981 4.19784247
Fe 11.52644683 11.30932121 4.15767111
Fe 12.67669800 12.22958924 9.85148310
S 10.58387312 12.25670672 10.76379315
Fe 9.26917672 12.11695644 4.15995019
Fe 7.06706178 12.34002826 5.49230047
Fe 12.51515048 8.02312791 9.93291938
S 10.51041995 7.80227938 10.84701042
Fe 8.95303538 8.08869495 4.29963081
Fe 6.88966619 8.24577094 5.58275618
Fe 7.57220425 13.57060645 7.67279696
Fe 8.85026929 13.55069836 9.94202506
Fe 7.30664671 6.99768684 7.76868203
Fe 8.56556276 7.03085377 10.08986304
Fe 11.00302514 13.43383204 5.49468093
Fe 12.21272652 13.43695628 7.61049849
Fe 10.65451598 6.78830690 5.57251361
Fe 11.97245655 6.80040640 7.74876914
C 8.61466861 14.04259568 11.85588060
C 11.19984849 14.08380567 11.92657358
C 9.88020332 14.23208480 12.57891201
C 6.40099123 12.83199240 11.78941917
C 7.45915331 13.49618460 12.57067394
C 5.52353010 10.44505012 11.49062502
C 5.79873687 11.63991712 12.31951993
C 6.22037593 8.01786697 11.91078142
C 5.71306933 9.28032622 12.37377273
C 8.32893848 6.65499341 12.03067542

C 7.22077419 7.31913126 12.72792114
C 10.89487377 6.52827290 12.09725847
C 9.57455946 6.42318832 12.76964055
C 12.99555834 7.85112478 11.89055622
C 12.06254232 7.17730517 12.76553768
C 14.01563754 10.14956851 11.58341433
C 13.67457428 8.98515401 12.44318916
C 13.14559564 12.52502289 11.77902336
C 13.73913003 11.37785141 12.37688874
C 12.26437346 13.33197570 12.61290404
C 6.84853931 9.00009650 14.59195594
C 7.49100188 9.74289871 15.66973470
C 6.07773387 9.76098416 13.68365502
C 6.12910080 11.19586796 13.65062639
C 7.54353297 11.20457948 15.63636530
C 6.95661179 11.94000186 14.51967567
C 8.90859660 7.76624844 16.01610531
C 8.43881775 7.13254333 14.84471740
C 7.36400879 7.71084741 14.12210502
C 8.49690114 9.05272398 16.41841709
C 10.86531300 8.96852684 16.44198781
C 11.92903480 9.58574412 15.71699783
C 9.70409389 9.74091715 16.86031894
C 11.97658399 11.05169928 15.68033040
C 9.75217281 11.10543545 16.83111099
C 10.96296101 11.77485964 16.37952724
C 13.36979403 9.49952008 13.74873517
C 13.40501149 10.94578174 13.70701509
C 10.79315089 7.05498157 14.85831592
C 9.59075745 6.58622179 14.15765598
C 10.36706674 7.70731000 16.02931284
C 11.92940416 7.55659603 14.15940192
C 12.53349654 8.79863406 14.64913984
C 12.62096174 11.74329395 14.57083647
C 12.10841355 13.00029953 14.02421785
C 8.59479829 11.85539960 16.35542227
C 11.02583109 13.61530027 14.70701971
C 9.86798496 14.12146604 13.97858881
C 10.55262718 13.04378612 15.90712820
C 9.09511982 13.09093194 15.89537781
C 8.67733084 13.69256740 14.68707299
C 7.56649053 13.16292796 13.98658452

$Fe_{49}S_6$ with nanocap(6,6)

Fe 9.90382317 10.03252945 12.97995465
Fe 12.02054505 10.04049263 13.90977668
Fe 10.03383747 9.99266779 15.54668378
Fe 9.89340739 10.00851294 10.72086789
Fe 7.86847210 10.00587066 11.95050779
Fe 9.24498839 11.94411747 11.92507842
Fe 10.51066551 12.03117647 14.00937631
Fe 9.25813978 8.08257052 11.98328227
Fe 10.61063745 8.03862897 13.93776344
Fe 8.24811286 8.81306576 14.05796088

Fe 8.16331487 11.28577138 14.01482278
Fe 11.54624446 8.84883787 11.89310329
Fe 11.51735644 11.27092862 11.93674478
Fe 14.34491515 10.13026936 14.99098157
S 12.22215493 10.02203974 16.04156602
S 10.18208304 9.84311241 17.95832735
Fe 9.92845477 9.95725565 8.27224334
Fe 7.80784867 9.92132655 9.53916212
Fe 5.70898304 9.85781435 10.78661797
Fe 8.65167033 14.01885071 10.74219483
Fe 9.79065544 14.04640311 12.97532672
Fe 10.74747564 14.14946658 15.25152220
Fe 8.56809022 5.97911660 11.04710078
Fe 9.94368219 5.96442701 13.05080046
Fe 11.27130546 5.84648846 15.13738711
Fe 6.34898879 7.91178711 15.30486737
Fe 6.28489244 10.31678669 15.21832186
Fe 6.15497572 12.74335213 14.58423233
Fe 13.27413364 7.56780101 10.83523046
Fe 13.30884793 10.08921854 10.78483506
Fe 13.24541935 12.60097441 10.95224111
S 8.27531443 8.55429765 16.19947159
S 8.32283384 11.17940943 16.16022385
Fe 13.76995779 8.83082057 12.88628203
Fe 13.75154274 11.32497598 12.94161093
Fe 6.09244752 8.80656968 13.02840671
Fe 6.03186334 11.22925595 12.78278299
Fe 11.61389206 8.76094474 9.49198464
Fe 11.59383503 11.29093380 9.54505671
Fe 12.77566742 12.09243442 15.15781078
S 10.80890270 12.11632739 16.14305597
Fe 9.27132461 11.98990890 9.51414836
Fe 7.14830608 11.95733383 10.71609548
Fe 12.84073816 7.98557660 15.11945431
S 10.78013091 7.93669675 16.05943898
Fe 9.23665046 7.95466511 9.59680205
Fe 7.09987715 7.90400816 10.92920895
Fe 7.50854439 13.29103073 12.75257842
Fe 8.47528448 13.40029690 15.21798289
Fe 7.54579865 6.78071303 13.18564315
Fe 8.97273732 6.66598161 15.32560737
Fe 10.95020212 13.35683160 10.85565790
Fe 12.18256006 13.36512134 13.08196134
Fe 10.93406918 6.72889769 10.85902301
Fe 12.30565155 6.74913222 12.94588870
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C 8.82730588 5.87541436 17.07060028
C 13.22249746 7.06525014 16.76903270
C 12.52587143 6.62032621 17.95273253
C 11.13812878 6.03028107 18.04868539
C 14.01909425 8.19893249 16.68351614
C 14.22642278 11.49355886 16.62135046
C 14.30038075 9.08068412 17.79548230
C 14.40544910 10.58699935 17.78296289
C 13.53505671 12.70879821 16.77182539

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C 11.66771422 13.85766614 18.16256529
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C 6.73387988 13.25539637 16.39236425
C 8.70106500 13.77505660 18.00174605
C 7.37324640 13.28429486 17.69866414
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C 5.61323250 8.92773050 16.92801153
C 5.76278691 9.98438840 17.91763748
C 5.91811227 11.40911748 17.64821556
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C 6.92482510 7.23025045 18.27376936
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C 9.23222768 10.03184483 21.24091425
C 13.78499801 9.19060833 20.24392629
C 14.00723783 10.56663264 20.25703929
C 12.68872132 8.62414738 20.99360416
C 11.66915543 9.46608212 21.54325367
C 11.93315699 10.86695705 21.56330494
C 13.16376316 11.37577205 21.07396611
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C 10.44863904 6.21619120 19.27787840
C 9.00969125 6.39977924 19.36994632
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Fe_{55} with CNT(10,0)

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Fe 7.74821169 10.07056268 6.56074461
Fe 9.13559493 12.05721168 6.56054756

Fe 10.40951917 12.12179228 8.61605437
Fe 9.20105589 8.14672648 6.56116487
Fe 10.49810186 8.13579030 8.60331009
Fe 8.14512094 8.85266886 8.61902860
Fe 8.08824325 11.31252988 8.60564757
Fe 11.48249028 8.93531276 6.54197264
Fe 11.43790876 11.35512440 6.55234129
Fe 14.04701533 10.15303677 9.45289796
Fe 11.95403934 10.45324346 10.96095184
Fe 9.81838721 10.14031966 12.19464545
Fe 9.77711760 10.12374433 2.83941468
Fe 7.66907260 10.08692125 4.11971959
Fe 5.58075399 10.04020821 5.40678891
Fe 8.45706934 14.12305929 5.41306625
Fe 9.73391656 14.16041729 7.49002472
Fe 11.08866179 14.16054913 9.56364081
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Fe 9.88763216 6.05574450 7.46618774
Fe 11.14721901 6.10039243 9.51026022
Fe 6.42765571 7.61270605 9.54759702
Fe 6.31799014 10.06459389 9.48481708
Fe 6.35627194 12.58428908 9.51080761
Fe 13.22027128 7.68314905 5.36026193
Fe 13.22112034 10.19077397 5.38334225
Fe 13.15358035 12.67659228 5.39538872
Fe 8.34465187 8.55947535 10.98488660
Fe 7.91831727 11.08826489 10.99170099
Fe 13.69284650 8.94837362 7.41024745
Fe 13.62931296 11.45668874 7.44029538
Fe 5.97990635 8.77074349 7.47712952
Fe 5.93889815 11.29622724 7.46523336
Fe 11.50476729 8.90980736 4.10936573
Fe 11.47015103 11.39702823 4.11689847
Fe 12.60437044 12.20545965 9.50253536
Fe 10.16388750 12.22801773 11.00253443
Fe 9.10245039 12.12372783 4.11827217
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Fe 12.66989090 8.10438116 9.45877965
Fe 10.84440147 8.20140454 10.96065711
Fe 9.15963748 8.10543915 4.13352819
Fe 7.04275024 8.04165265 5.42321550
Fe 7.36292602 13.34891665 7.47151937
Fe 8.68713376 13.41183976 9.51149248
Fe 7.48774192 6.79073552 7.48974630
Fe 8.79190249 6.77573520 9.54187232
Fe 10.79736858 13.41717468 5.41166474
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Fe 12.23720709 6.87276129 7.43348099
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C 7.70984970 7.45512722 20.78901370
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Fe_{55} with CNT(6,6)

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Fe 9.33955428 11.90595664 8.92288824
Fe 10.61410509 11.88054021 10.99256841
Fe 9.14250610 8.00754515 8.98618336
Fe 10.41076460 7.97130522 11.04326348
Fe 8.09608882 8.81066209 10.98350219
Fe 8.23143993 11.28752927 10.93636005
Fe 11.45544703 8.65034037 8.96384434
Fe 11.57454925 11.03969913 8.93584625
Fe 14.32603712 9.71342878 11.79580178
Fe 11.75356751 9.87045309 13.44258505
Fe 9.71672006 10.05170447 14.74110747
Fe 9.85006665 9.87856663 5.22506932
Fe 7.78537087 9.97812886 6.48967349
Fe 5.66784322 10.08782488 7.75575646
Fe 8.77001896 13.98754581 7.77008538
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Fe 11.40291153 13.96669784 11.82358754
Fe 8.37866365 5.95289783 7.89181803
Fe 9.67286428 5.89212307 9.92251974
Fe 10.96044067 5.83908484 11.91917078
Fe 6.23325092 7.73863490 12.06628564
Fe 6.30784265 10.16937574 11.69642040
Fe 6.52457531 12.61056119 11.97264058
Fe 13.15797768 7.29282434 7.79391357
Fe 13.29173988 9.74890229 7.81641098
Fe 13.39479700 12.20772847 7.74376455
Fe 8.00189311 8.90729448 13.45506189
Fe 8.17833772 11.34075368 13.40460721
Fe 13.62312319 8.49338459 9.89847745
Fe 13.75094003 10.98321480 9.87375287
Fe 5.93607990 8.83510549 9.78885984
Fe 6.06625294 11.43649726 9.72240548
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Fe 11.65040102 11.04804404 6.50237406
Fe 12.85793494 11.74765377 12.11368631
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Fe 12.63688320 7.86528297 12.15510903
Fe 10.25596954 7.81190456 13.44525384
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Fe 7.05982657 8.01401515 7.77620665
Fe 7.61801290 13.34232987 9.80964910
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Fe 7.27642648 6.77919697 9.92982505
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C 6.73160802 13.12303036 19.57556299
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C 5.85399174 11.99024368 19.55520878
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C 5.87167185 9.98645902 20.97609692
C 5.87756820 11.39749207 20.84487039
C 6.67239063 7.90779629 19.86701105
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$Fe_{54}S$ with CNT(10,0)

Fe 9.80924202 10.11697086 7.51115261
Fe 11.89647364 10.17460487 8.54368693
Fe 9.82181614 10.11357896 9.79556689
Fe 9.78761713 10.12800396 5.21470764
Fe 7.75672598 10.05207259 6.52919810
Fe 9.10972605 12.04499347 6.52424125
Fe 10.40061348 12.10862859 8.55771287
Fe 9.23734521 8.14777654 6.50695156
Fe 10.51843094 8.16213992 8.56532604
Fe 8.18072693 8.82836015 8.56346264
Fe 8.10394531 11.28069664 8.56203969
Fe 11.49098527 8.96515831 6.49079208
Fe 11.42156379 11.37601281 6.50136837
Fe 14.07242143 10.20602018 9.45760827
Fe 11.97738889 10.41663874 10.93682769
S 9.84687338 10.11236147 12.03297984
Fe 9.75673549 10.14864441 2.87108397
Fe 7.63757131 10.04965511 4.15254212
Fe 5.56368678 9.95515678 5.36113861
Fe 8.37709307 14.11275971 5.34527586
Fe 9.69949178 14.15981133 7.46882623
Fe 11.10501270 14.14151032 9.56644012
Fe 8.66922226 6.04279777 5.31936106
Fe 9.92275842 6.08361981 7.41909309
Fe 11.13958462 6.11334696 9.53379901
Fe 6.42704843 7.57832169 9.55437926
Fe 6.33087716 10.01255378 9.52665489
Fe 6.37419286 12.57456005 9.51248702
Fe 13.25388797 7.70351186 5.31575764
Fe 13.19795283 10.22269288 5.35906019
Fe 13.13974733 12.71035863 5.30149284
Fe 8.26683278 8.61114982 10.98545713
Fe 7.90813084 11.12017255 10.96635276
Fe 13.67251446 8.96692132 7.41526601
Fe 13.61086995 11.47670878 7.38437283
Fe 5.99905269 8.74538845 7.44443546
Fe 5.91673868 11.24657025 7.45779276
Fe 11.54773886 8.95190489 4.10612887
Fe 11.44691220 11.46054776 4.11300723
Fe 12.59928798 12.24691848 9.52457000
Fe 10.20445318 12.24312253 10.97551938
Fe 9.03426632 12.13893071 4.14563280
Fe 6.96495162 12.03482926 5.43142586
Fe 12.67247978 8.14211382 9.46878047
Fe 10.75611369 8.16445893 10.97991290
Fe 9.19780468 8.08703049 4.11210669
Fe 7.12332886 8.00590559 5.41413009

Fe 7.35632520 13.34248665 7.43702598
Fe 8.65688738 13.41377097 9.55393640
Fe 7.54983271 6.75349839 7.45283195
Fe 8.81553744 6.74783618 9.56977452
Fe 10.74721367 13.40243549 5.41279194
Fe 12.12053747 13.45977732 7.42546884
Fe 10.95658858 6.90188077 5.35067946
Fe 12.26344078 6.93486444 7.44297462
C 13.00803311 12.27098897 11.43679751
C 13.89637697 9.99057561 11.38901023
C 13.66514711 11.20671114 12.15193086
C 11.19676803 13.91687365 11.51262591
C 12.23167179 13.20535250 12.23227566
C 8.76155447 13.80859423 11.46789795
C 9.95298519 14.05608395 12.24801940
C 6.61884226 12.59715175 11.44124608
C 7.58962210 13.36996532 12.19376322
C 5.96514688 10.22885308 11.42472345
C 6.05385412 11.46876210 12.16530461
C 6.48244748 7.82137917 11.49499157
C 6.02796560 9.00131982 12.19816612
C 8.52538394 6.49354647 11.49509669
C 7.40560092 6.99380155 12.25486333
C 10.95683766 6.21898477 11.46741046
C 9.72952523 6.18878852 12.24089641
C 12.86906673 7.75326397 11.37829795
C 12.07758410 6.82846538 12.15689607
C 13.59998604 8.76701556 12.11422724
C 12.24814117 13.17172709 13.66141655
C 13.68847460 11.18252362 13.59012295
C 13.11118533 12.24974641 14.34291345
C 9.93697185 13.99294971 13.69011264
C 11.14917020 13.73143727 14.40956423
C 7.55457943 13.39572027 13.61833560
C 8.69434223 13.84038422 14.37306496
C 6.01269398 11.48214813 13.59559372
C 6.59061477 12.58693092 14.30647497
C 5.98449160 9.02086862 13.62379584
C 5.78636727 10.26168371 14.30734945
C 7.43943117 7.04961075 13.69718858
C 6.55618280 7.93858369 14.38411872
C 9.74889282 6.20583358 13.67051100
C 8.55353179 6.50678661 14.41212844
C 12.11705351 6.83575278 13.59577318
C 11.00586950 6.34474034 14.35399750
C 13.69300138 8.72731054 13.52828404
C 13.07712664 7.64723905 14.25787814
C 13.94634363 9.94940075 14.25735359
C 11.13062581 13.65317851 15.83527186
C 13.12481855 12.20409291 15.77244098
C 12.23649705 13.03928970 16.53011859
C 8.66935396 13.80798756 15.80283052
C 9.89477534 13.87841383 16.54569547
C 6.53606159 12.61114873 15.72021408
C 7.48369228 13.38169434 16.48343866

C 5.71609721 10.28328151 15.72433744
C 5.83202251 11.55137218 16.38913801
C 6.57168243 7.99257721 15.81001896
C 5.94510998 9.08853211 16.48948482
C 8.58362602 6.56677630 15.84287147
C 7.48342458 7.16926479 16.55295319
C 11.04153380 6.38963781 15.77904676
C 9.82295888 6.32423402 16.53863531
C 13.16276342 7.61002418 15.67351387
C 12.22937672 6.83556916 16.44501439
C 14.01653667 9.92403150 15.66940342
C 13.89325226 8.65454350 16.33552688
C 13.77341105 11.11621399 16.43955493
C 9.87484836 13.82801312 17.97528931
C 12.23333537 12.98057681 17.95755213
C 11.12419079 13.58604703 18.65979053
C 7.46062417 13.33776751 17.91890934
C 8.63132627 13.65989864 18.69144097
C 5.75603167 11.58136827 17.77507466
C 6.45384644 12.56501958 18.54931298
C 5.95811051 9.14298488 17.92483629
C 5.67347398 10.38077225 18.55185326
C 7.50315415 7.22569427 17.98309665
C 6.65344272 8.14996910 18.69902454
C 9.85834860 6.37467586 17.96650643
C 8.62010679 6.62006803 18.66903882
C 12.26905751 6.87476658 17.88137974
C 11.11125093 6.54714215 18.66792396
C 13.98004175 8.62413019 17.71909586
C 13.28382340 7.64433758 18.49892538
C 13.77746516 11.06177360 17.87582969
C 14.07424342 9.82455686 18.49797331
C 13.09020618 12.05175493 18.65952627
C 6.70138984 9.70047938 20.70227601
C 7.54514517 10.16660726 21.79518057
C 6.14290522 10.68253371 19.86607269
C 6.62817553 12.03592148 19.86345652
C 8.03929144 11.54551219 21.79314201
C 7.68391788 12.44055732 20.69916630
C 8.30780050 7.84108849 22.02336071
C 7.69357612 7.46197835 20.80549650
C 6.85307611 8.36960306 20.12128878
C 8.30741294 9.17568922 22.48823171
C 10.54037711 8.37145892 22.47506273
C 11.74984786 8.65293354 21.76862721
C 9.67162972 9.45399423 22.92588794
C 12.24583709 10.03211425 21.76625500
C 10.13463880 10.74268322 22.92357208
C 11.49275137 11.02210858 22.46982944
C 13.13116408 8.16917984 19.81713789
C 13.62103200 9.52160027 19.81607400
C 9.89811504 6.66781058 20.79077595
C 8.64697905 6.66741825 20.06490895
C 9.68175119 7.34647494 22.01346766
C 11.11550481 6.83586737 20.09118308

C 12.08780687 7.76204998 20.66560272
C 13.07228058 10.50163848 20.66214160
C 12.91161301 11.83206265 20.08429433
C 9.25916318 11.82521771 22.48436129
C 12.08034562 12.73922113 20.78078879
C 11.11559434 13.53596133 20.05447467
C 11.48432571 12.35769793 22.00491917
C 10.10919462 12.85113717 22.01444988
C 9.87472009 13.53373766 20.79687735
C 8.64679720 13.36957904 20.11545158

$Fe_{54}S$ with CNT(6,6)

Fe 9.88705642 9.91919386 9.92145335
Fe 11.94309027 9.85652082 10.99790256
Fe 9.80618708 9.96298999 12.23515429
Fe 9.88101073 9.90156551 7.65367394
Fe 7.84683894 9.96714432 8.91106506
Fe 9.31707682 11.87907423 8.91434081
Fe 10.60224374 11.86713664 10.97628833
Fe 9.20302393 7.97778302 8.95260348
Fe 10.46997685 7.96321942 11.01754092
Fe 8.15495153 8.76045243 10.97821409
Fe 8.23307179 11.21922282 10.94801986
Fe 11.49543088 8.66725423 8.92809699
Fe 11.57061306 11.05299445 8.90623139
Fe 14.30809462 9.74388201 11.80767445
Fe 11.85049431 9.88874823 13.41363297
S 9.75322606 10.01665681 14.47661591
Fe 9.83160340 9.89653622 5.21837229
Fe 7.77392354 9.93350479 6.49618304
Fe 5.67039264 9.98929693 7.78828480
Fe 8.71241352 13.96497678 7.78375356
Fe 10.04768837 13.97431433 9.81232872
Fe 11.37630398 13.95729606 11.83069254
Fe 8.51142602 5.90200786 7.84493878
Fe 9.79369778 5.87383081 9.89125293
Fe 11.04520568 5.84096067 11.93800113
Fe 6.31838607 7.56267110 12.00495153
Fe 6.32456365 10.02655159 11.76220476
Fe 6.50099530 12.52189524 11.97498632
Fe 13.21809804 7.34088825 7.76306088
Fe 13.30357208 9.79732554 7.77040894
Fe 13.36609917 12.24936293 7.72233885
Fe 7.96081632 8.83570449 13.42628041
Fe 8.13124911 11.31023629 13.39125878
Fe 13.66780932 8.53453056 9.86970872
Fe 13.75707107 11.01073447 9.84605327
Fe 6.00043326 8.73625415 9.80538491
Fe 6.06442883 11.32381669 9.76399799
Fe 11.56205299 8.60913077 6.49749018
Fe 11.62519317 11.08545297 6.47372697
Fe 12.86615840 11.77582766 12.11523369
Fe 10.55094627 12.14532840 13.35595489
Fe 9.32337125 11.93180930 6.49844510

Fe 7.21988323 11.98189570 7.72223669
Fe 12.67807012 7.86949729 12.17318679
Fe 10.30105587 7.80298205 13.42514858
Fe 9.22525136 7.88677019 6.53455404
Fe 7.10648239 7.93474369 7.77188999
Fe 7.57562268 13.27805185 9.81138817
Fe 8.96153032 13.34693164 11.81613831
Fe 7.39625139 6.70005263 9.90121436
Fe 8.72333306 6.65587789 11.93179323
Fe 11.08274871 13.12192308 7.80269380
Fe 12.43147024 13.01948326 9.92083673
Fe 10.89643301 6.61394010 7.85787425
Fe 12.20742820 6.65818599 9.98717681
C 11.16384202 5.97923614 13.82253069
C 12.35426631 6.73427125 13.75209703
C 13.71897384 9.03340694 13.63986279
C 13.81486477 10.48890148 13.62454871
C 12.77823211 12.93714916 13.67946210
C 11.71609446 13.84751155 13.70324643
C 8.95642196 13.90149446 13.60930131
C 7.65260288 13.35147110 13.49162348
C 6.03457787 11.02237080 13.49143628
C 5.93713606 9.58523602 13.58336454
C 8.36957519 6.37049193 13.78177870
C 7.09917628 7.00069681 13.72276007
C 10.43577510 5.92416447 15.05230854
C 9.00888443 6.09188551 15.03059970
C 12.99143487 7.13746531 14.97465069
C 11.15559846 6.11266248 16.26979328
C 12.46850736 6.68868160 16.22549278
C 13.74139583 8.35240551 14.92266243
C 13.92657646 11.18540028 14.89154886
C 14.04824854 9.04637319 16.12799685
C 14.13567824 10.48191213 16.11168468
C 13.34116879 12.48570542 14.91962834
C 11.02011449 14.09360997 14.93114966
C 12.87274283 13.03251438 16.15218757
C 11.66874773 13.81625434 16.17101883
C 9.58773823 14.16019198 14.86587402
C 7.04222195 12.93278751 14.73710101
C 8.83550831 14.03433730 16.07358080
C 7.54186898 13.42988125 15.99052491
C 6.22120168 11.74322561 14.72743444
C 5.99895876 8.92200885 14.85354962
C 5.92250492 11.10705997 15.98111514
C 5.83005811 9.68633826 16.05837302
C 6.63434558 7.62646595 14.94680264
C 8.32526349 6.38941429 16.25553017
C 7.14134299 7.18785685 16.21875080
C 10.43937980 6.07864794 17.50507463
C 9.00918575 6.22388485 17.50289398
C 13.02782415 7.20652266 17.43506576
C 11.16050933 6.22703247 18.72209191
C 12.48376552 6.79003029 18.68564068
C 13.85056283 8.38203645 17.38751658

C 14.00830704 11.19487758 17.35223493
C 14.13678942 9.06973275 18.60328023
C 14.21746984 10.50582314 18.58658546
C 13.33058455 12.45651854 17.37407328
C 10.93655518 13.97098623 17.39509467
C 12.81904496 12.95094750 18.61405318
C 11.57967306 13.67878510 18.64092610
C 9.51145644 14.11408026 17.35148626
C 6.89819501 13.02662275 17.18926229
C 8.76049301 13.97854026 18.56285471
C 7.39478159 13.53416613 18.43928101
C 6.06023315 11.86045416 17.18048672
C 5.96115447 9.04533446 17.34034695
C 5.69843467 11.23885608 18.42051561
C 5.73100391 9.79857312 18.53155038
C 6.66083195 7.79583454 17.42311640
C 8.34146255 6.53679077 18.72573197
C 7.14404340 7.34180605 18.69386020
C 10.45435343 6.14389153 19.96455034
C 9.02571152 6.31711417 19.96778589
C 13.09451048 7.24579425 19.89715930
C 12.55549510 6.79300977 21.14727721
C 11.21124786 6.24202766 21.18193221
C 13.94908326 8.39987455 19.85715654
C 14.12445076 11.23035735 19.81326048
C 14.28622706 9.09435631 21.07118701
C 14.39745296 10.54374138 21.04828116
C 13.37454591 12.45851510 19.82669153
C 10.85490701 13.78784466 19.87833714
C 12.86910312 12.96997182 21.06810776
C 11.52639974 13.50262906 21.11525633
C 9.42265818 13.90791733 19.84798393
C 6.71157456 13.14932176 19.59152436
C 8.67425232 13.54815069 21.04006810
C 7.31155502 13.21938439 20.88500669
C 5.82969907 12.01818821 19.57867685
C 5.93192427 9.19204483 19.82391217
C 5.84661795 10.02204011 21.00875492
C 5.85371142 11.43183016 20.87182247
C 6.64790815 7.94052451 19.90237768
C 7.16349219 7.47135773 21.17031827
C 8.34311116 6.62103293 21.19747122
C 7.90355304 9.54315050 23.95737609
C 7.72284583 8.19105136 23.49101299
C 6.32764136 9.53063242 22.24053989
C 6.85944119 8.20755051 22.34430223
C 7.01406407 10.36901441 23.19465284
C 9.99515892 7.69452470 24.21100803
C 8.78069931 7.31160189 23.55498856
C 10.22686444 9.03600671 24.64131336
C 9.15491204 10.01231477 24.41646941
C 13.78500464 9.22138889 23.51840121
C 13.98574903 10.60123217 23.50760812
C 12.66250977 8.65160011 24.22877822
C 11.61186310 9.48691222 24.74055180

C 11.85902504 10.89748460 24.74143325
C 13.09020899 11.41926806 24.26650345
C 13.98165221 8.46394289 22.30022584
C 14.25576608 11.26733926 22.25068767
C 11.04439562 6.94118387 23.56561046
C 10.49549608 6.28848770 22.39622825
C 9.07974643 6.49785544 22.39920273
C 13.10810178 7.32728634 22.33114792
C 12.33431787 7.42570311 23.54414908
C 9.49511609 11.40402698 24.09703216
C 10.81178045 11.82291204 24.32526969
C 7.38142071 11.68725476 22.82446664
C 6.69904164 12.23316682 21.71821695
C 13.48800161 12.50209247 22.25306173
C 8.68991151 12.18405003 23.16669816
C 10.75755603 13.30842355 22.33378028
C 12.81611860 12.60679451 23.49220310
C 11.41726678 12.84035440 23.49645299
C 9.33865427 13.11109310 22.24977929

$Fe_{52}S_3$ with CNT(10,0)

Fe 9.82073436 10.16280927 7.60067649
Fe 12.00693162 10.06991729 8.52443678
Fe 9.69967663 10.18526274 9.98608596
Fe 9.77194960 10.18960871 5.30306666
Fe 7.74654972 10.19879385 6.63274351
Fe 9.17403077 12.12965027 6.59907970
Fe 10.48256343 12.21444380 8.59387399
Fe 9.17720565 8.20525003 6.62311535
Fe 10.50335148 8.16694095 8.71610622
Fe 8.11398778 8.94801773 8.63866491
Fe 8.14192275 11.45782018 8.71730327
Fe 11.42664823 8.92384474 6.50111715
Fe 11.49111493 11.35637580 6.55362997
Fe 14.08831872 10.01749171 9.44422016
S 11.53063715 11.29346477 10.37847819
Fe 11.88374330 9.22780558 10.83499151
Fe 9.73337421 10.20258114 2.93789369
Fe 7.63882528 10.19107181 4.22235599
Fe 5.55998012 10.16815869 5.40354972
Fe 8.52569938 14.22565842 5.36871807
Fe 9.84897090 14.28185425 7.42823557
Fe 11.23331394 14.16632336 9.51603969
Fe 8.47515399 6.11506610 5.45777504
Fe 9.73352473 6.10367955 7.50599519
Fe 10.95814426 6.03507538 9.60159773
Fe 6.42292027 7.65520139 9.55921270
Fe 6.26374874 10.21015153 9.45809647
Fe 6.40414299 12.68270651 9.49393186
Fe 13.08860447 7.58024636 5.22695257
Fe 13.17619457 10.09510391 5.35731784
Fe 13.26432065 12.61127370 5.32776854
Fe 7.78010073 9.33134440 10.98977614
S 9.09538387 10.70008480 12.15974373

Fe 13.67175453 8.74773653 7.31812879
Fe 13.75932132 11.34099331 7.34091692
Fe 5.92225182 8.92022543 7.48250939
Fe 5.93352677 11.47192049 7.43484707
Fe 11.45367302 8.92633092 4.10588859
Fe 11.50167330 11.41544887 4.16431373
Fe 13.07256533 12.39720266 9.43542201
Fe 9.78056276 12.41078990 10.93364321
Fe 9.14038694 12.22041758 4.19026487
Fe 7.03813437 12.20860902 5.41770541
Fe 12.79730116 7.78160729 9.39204264
S 9.83636841 8.23758269 10.88691444
Fe 9.09915461 8.18595724 4.20924794
Fe 7.06179496 8.17828020 5.49560086
Fe 7.41820114 13.49294717 7.40484742
Fe 8.67810574 13.68223304 9.43218772
Fe 7.39296710 6.84675320 7.52801109
Fe 8.68211373 6.72475789 9.73033142
Fe 10.87084072 13.38882463 5.43765447
Fe 12.28819289 13.46144725 7.37950896
Fe 10.77639330 6.83235859 5.30536395
Fe 12.03228437 6.83323598 7.35471067
C 13.16852689 12.40611166 11.44614285
C 13.73240085 9.93042375 11.38671895
C 13.63575628 11.21321284 12.12350768
C 11.11697846 13.86735880 11.46616433
C 12.25040956 13.25549552 12.19007598
C 8.63216525 13.96701538 11.40887683
C 9.87463900 14.10393464 12.19403797
C 6.58726787 12.53937502 11.39588685
C 7.48973842 13.39343695 12.12151310
C 5.97330956 10.11497754 11.38801181
C 6.08378480 11.39069675 12.10212278
C 6.67401557 7.72730054 11.49969584
C 6.09318325 8.88120660 12.17274101
C 8.52861991 6.08593992 11.57406649
C 7.48635881 6.78348608 12.27941962
C 10.99222351 5.92872245 11.54783508
C 9.75248782 5.81946265 12.30463024
C 12.90050342 7.56593744 11.38488956
C 12.07504899 6.62977171 12.17942557
C 13.52456848 8.68198825 12.11571129
C 12.20829477 13.18874787 13.61226839
C 13.63590550 11.17933572 13.54562360
C 13.06757898 12.26462815 14.30135781
C 9.86791943 13.99837100 13.63282533
C 11.07995437 13.72215077 14.34708154
C 7.49518145 13.36870020 13.55301581
C 8.62203168 13.84384575 14.31266432
C 6.02931529 11.39389391 13.52173584
C 6.58132949 12.51030398 14.23904093
C 6.09409944 8.92357738 13.61098628
C 5.83883275 10.16362912 14.26039136
C 7.48425515 6.87599665 13.70588975
C 6.64073343 7.83941412 14.37141706

C 9.77220675 5.97168881 13.73066892
C 8.57546130 6.31555680 14.45628452
C 12.11669883 6.69788966 13.61117822
C 11.02236665 6.19510479 14.39960431
C 13.56320062 8.69858767 13.54630137
C 13.02697113 7.58812687 14.27554318
C 13.82141173 9.93022882 14.23588537
C 11.06075079 13.65305861 15.77438015
C 13.06167185 12.21614621 15.72655237
C 12.16920970 13.05367669 16.47898896
C 8.60142599 13.79785978 15.73848993
C 9.82478276 13.87910949 16.48185231
C 6.51229219 12.54004606 15.65442731
C 7.42664913 13.34145312 16.41851630
C 5.75013287 10.19542634 15.67308728
C 5.82649358 11.47228881 16.32755332
C 6.62891216 7.90812332 15.79811278
C 5.98971146 9.01070116 16.45355264
C 8.60186346 6.43378289 15.88006807
C 7.50796098 7.07353463 16.57017536
C 11.05550981 6.28724664 15.82535278
C 9.84026752 6.21917053 16.58795170
C 13.12375242 7.57891629 15.68921957
C 12.22714372 6.78146923 16.48292782
C 13.91558079 9.92345611 15.64867279
C 13.81720567 8.66187755 16.32964467
C 13.69933022 11.12827356 16.40698957
C 9.80287034 13.83479733 17.91154793
C 12.16543396 13.00645370 17.90596881
C 11.05154774 13.61026044 18.60130197
C 7.39934047 13.30481629 17.85279852
C 8.56059238 13.65268132 18.62640544
C 5.73489150 11.51392571 17.71033467
C 6.40523295 12.51724105 18.48162703
C 5.97540041 9.07805233 17.88982147
C 5.66578617 10.31874359 18.49874828
C 7.51544923 7.15808166 17.99697141
C 6.66271322 8.09939514 18.68852442
C 9.87071052 6.31245776 18.01371696
C 8.62799923 6.56734485 18.70496987
C 12.26699951 6.85516999 17.91635304
C 11.11777143 6.52238833 18.71378694
C 13.92522676 8.65054165 17.71406909
C 13.26117056 7.66651645 18.51620103
C 13.71159955 11.09093192 17.84136509
C 14.01240099 9.86058560 18.47583295
C 13.02520579 12.08799307 18.61846127
C 6.67423831 9.67914447 20.66983302
C 7.50331170 10.17249867 21.76239538
C 6.11294924 10.64218912 19.81442389
C 6.57797512 12.00390342 19.80208290
C 7.98275104 11.55716948 21.74581737
C 7.62120365 12.43513773 20.63955699
C 8.28975812 7.85855116 22.03200498
C 7.68582847 7.45217158 20.81817180

C 6.84496617 8.34201220 20.10973943
C 8.27279114 9.20128188 22.47389273
C 10.51378789 8.42248457 22.48195047
C 11.71967516 8.70852437 21.77099368
C 9.63201086 9.50206817 22.91283654
C 12.19869311 10.09337442 21.74852702
C 10.08065174 10.79531990 22.89502621
C 11.43673371 11.08449472 22.44022008
C 13.10551196 8.20938807 19.82595692
C 13.57399843 9.57062451 19.80224909
C 9.89739441 6.67873165 20.83011446
C 8.64906989 6.64989280 20.09842871
C 9.66918359 7.37754440 22.03867911
C 11.11434894 6.84712179 20.12973526
C 12.07028780 7.80179158 20.68433555
C 13.02034275 10.55590516 20.63689518
C 12.84771374 11.88012373 20.04448282
C 9.19507854 11.86129183 22.43877093
C 12.00956920 12.78814982 20.73211873
C 11.04016690 13.57036016 19.99610270
C 11.41514629 12.41503831 21.95992464
C 10.03520637 12.89269290 21.95964493
C 9.79735312 13.55975016 20.73455244
C 8.57428138 13.37245894 20.05123766

$Fe_{52}S_3$ with CNT(6,6)

Fe 9.82587604 9.99978052 10.00557387
Fe 11.90833904 10.01288230 11.07963034
Fe 9.64551405 10.18075545 12.42725333
Fe 9.85823500 9.92434912 7.74726922
Fe 7.79619946 9.91785948 8.97034251
Fe 9.16931659 11.89597333 8.92360120
Fe 10.40284494 12.02011384 10.99250073
Fe 9.24923399 8.00385520 9.07068167
Fe 10.55005546 8.07884362 11.12966211
Fe 8.15357628 8.79199462 11.06845648
Fe 8.09464098 11.23237547 10.93623478
Fe 11.52399692 8.79188720 9.01996985
Fe 11.47100275 11.20492813 8.99129417
Fe 14.10852540 10.12049077 11.89144212
S 11.70976628 10.60132856 13.18008692
Fe 10.76850290 9.44882249 14.84322345
Fe 9.87547019 9.86161008 5.27918097
Fe 7.78339924 9.80830298 6.53948830
Fe 5.63376638 9.81834324 7.77709152
Fe 8.46319247 13.91699441 7.69350243
Fe 9.76731417 14.06498261 9.69567112
Fe 11.01315748 14.17453795 11.86719327
Fe 8.65146497 5.86166424 8.03091196
Fe 9.91903508 5.97953843 10.08762856
Fe 11.22147879 6.00548439 12.04182651
Fe 6.35871733 7.50594905 12.02136735
Fe 6.24433384 9.99103369 11.71995562
Fe 6.40877060 12.43972111 11.95248089

Fe 13.30363130 7.51550896 7.86676430
Fe 13.28391596 10.00666650 7.88774390
Fe 13.23418650 12.48896237 7.85764126
Fe 7.87831980 8.92857406 13.51877270
S 8.94032711 10.72272502 14.57312280
Fe 13.71606500 8.78041745 9.92672188
Fe 13.62506786 11.31102806 9.93869639
Fe 5.98703863 8.62598664 9.81497761
Fe 5.91024332 11.22048481 9.71064795
Fe 11.60956880 8.67752445 6.59186067
Fe 11.56294886 11.13537944 6.57393394
Fe 12.60950716 12.18481004 11.95518222
Fe 10.23988811 12.30324442 13.43951957
Fe 9.20934019 11.87089484 6.48979756
Fe 7.08454749 11.85019987 7.66978346
Fe 12.82972760 7.95493758 12.16551691
S 9.97879726 8.12100080 13.23921182
Fe 9.30156994 7.86651372 6.65907032
Fe 7.16458725 7.82991464 7.85767394
Fe 7.31822120 13.24630233 9.68731116
Fe 8.64278304 13.42054795 11.66964211
Fe 7.48833424 6.66775480 10.02896874
Fe 8.76938931 6.69001568 12.11406130
Fe 10.86994575 13.18430449 7.73221291
Fe 12.13295395 13.35303813 9.86291092
Fe 10.98182558 6.67462015 7.97409822
Fe 12.30161262 6.77358078 10.00097042
C 11.19649360 5.74594225 13.88236759
C 12.36127238 6.50490957 13.73602528
C 14.08194069 8.95156933 13.63998379
C 14.39955531 10.31206017 13.71214553
C 13.09157010 12.96830824 13.60351608
C 11.86903784 13.68589628 13.56076607
C 8.93719682 13.95356868 13.46944703
C 7.62371393 13.40912437 13.38988270
C 5.94192233 11.00673341 13.42043476
C 5.87980560 9.58516033 13.53400916
C 8.25651654 6.02981014 13.80966479
C 7.15447928 6.91874416 13.72136395
C 10.39353783 5.71858255 15.05036361
C 8.95042467 5.84377867 15.03124695
C 12.91648655 7.10338374 14.91393260
C 11.09444855 6.04621049 16.25246465
C 12.37064066 6.69656346 16.18792540
C 13.76082855 8.28053396 14.86799261
C 14.20788651 11.12455983 14.85709575
C 14.03380931 8.98078549 16.09736568
C 14.22544400 10.40164710 16.08820441
C 13.57323690 12.42513812 14.82123212
C 11.09433448 13.87901469 14.77082666
C 12.96895391 12.90492434 16.04343509
C 11.73006687 13.62086888 16.03417879
C 9.65234109 14.04029638 14.71512897
C 6.99870040 12.96155646 14.59895752
C 8.88844173 13.93031786 15.93294054

C 7.55341096 13.42092256 15.84750647
C 6.15680683 11.77695468 14.61049559
C 6.04304981 8.91757701 14.79575424
C 5.90244869 11.13314313 15.87159640
C 5.86669490 9.70773007 15.98560825
C 6.70323687 7.62735382 14.90210846
C 8.30039496 6.29954472 16.24059088
C 7.17322751 7.17740511 16.18725499
C 10.39528273 6.02013874 17.50301816
C 8.97002300 6.16759729 17.49931446
C 12.94915686 7.18746083 17.40436727
C 11.11631007 6.19292891 18.71259310
C 12.43771126 6.75647878 18.66442544
C 13.80207330 8.33558593 17.35913909
C 14.08178977 11.11957577 17.31547428
C 14.12998653 9.00558223 18.57307174
C 14.25359665 10.43725073 18.54935663
C 13.41068517 12.37885245 17.29406367
C 10.99534128 13.83219227 17.24967849
C 12.87571154 12.88616588 18.51519371
C 11.63201781 13.60041825 18.51335160
C 9.57007166 13.99937039 17.20238675
C 6.91427361 13.03836606 17.06321388
C 8.81822056 13.92893303 18.42050403
C 7.43905953 13.53239976 18.30575459
C 6.06006674 11.88880864 17.07214523
C 6.00208815 9.07627629 17.26986027
C 5.71388811 11.27282378 18.32025198
C 5.74933935 9.83459990 18.45196689
C 6.68606210 7.81591639 17.37385185
C 8.30533107 6.52829340 18.70956014
C 7.12909481 7.35954275 18.65758413
C 10.41033579 6.13188243 19.95705792
C 8.98424504 6.32200921 19.95525801
C 13.05926440 7.20768572 19.87379842
C 12.51769130 6.77240044 21.13201769
C 11.16644206 6.23940110 21.17395013
C 13.93037642 8.34907117 19.82970896
C 14.15838385 11.17898203 19.76082749
C 14.27996264 9.05079125 21.03836179
C 14.41122890 10.49937638 21.00274258
C 13.42145812 12.41317855 19.74233793
C 10.90525608 13.74488821 19.74832853
C 12.90826646 12.94331331 20.97118034
C 11.56869963 13.48357764 20.99804615
C 9.47575678 13.87479010 19.70886157
C 6.75056544 13.17759821 19.46689549
C 8.72020624 13.55602211 20.90868886
C 7.35312708 13.25235975 20.75984269
C 5.85441674 12.06223141 19.47054421
C 5.93520152 9.23983070 19.75258669
C 5.84936348 10.08372159 20.92766167
C 5.86963261 11.49081913 20.77321101
C 6.63387483 7.98106299 19.85447508
C 7.13495600 7.52108871 21.13222153

C 8.30220798 6.65459109 21.17728065
C 7.88990141 9.61671787 23.89388004
C 7.69325835 8.26111895 23.44642209
C 6.32076037 9.60322599 22.16872051
C 6.83474281 8.27447806 22.29577835
C 7.01238977 10.44438964 23.11469671
C 9.95862301 7.74464949 24.18099603
C 8.74144716 7.36973165 23.52622335
C 10.20640122 9.08863246 24.59172588
C 9.14585967 10.07482165 24.34934197
C 13.77183621 9.21459230 23.48035358
C 13.98920828 10.59288607 23.45424151
C 12.63913431 8.66816561 24.19250839
C 11.59676069 9.52331442 24.69013347
C 11.85992681 10.93061690 24.67184493
C 13.09696887 11.43128316 24.19324145
C 13.96316037 8.43940769 22.27223695
C 14.27166204 11.24024963 22.19133976
C 11.00104210 6.96838102 23.54845147
C 10.44791094 6.31000210 22.38583854
C 9.03464783 6.53919742 22.38169455
C 13.07295321 7.31464421 22.31159126
C 12.29697844 7.43780466 23.52165289
C 9.50376198 11.45673571 24.00863390
C 10.82348401 11.86167274 24.23429636
C 7.39609168 11.75279515 22.72708419
C 6.72307301 12.29167684 21.61073836
C 13.51630883 12.48397828 22.16673249
C 8.71093828 12.23422387 23.06371707
C 10.79376082 13.31851502 22.21818566
C 12.83814824 12.61043742 23.39888044
C 11.44284545 12.85927261 23.39109807
C 9.37384611 13.13452576 22.13149443

$Fe_{49}S_6$ with CNT(10,0)

Fe 9.79325393 10.09740391 7.35298828
Fe 11.88757826 10.08171697 8.32471554
Fe 9.76239583 10.02587263 9.76846901
Fe 9.78360863 10.10984582 5.09620346
Fe 7.74475322 10.12733578 6.33140412
Fe 9.18936511 12.05704544 6.33943084
Fe 10.47233742 12.05775777 8.36918780
Fe 9.13828053 8.16772214 6.31267994
Fe 10.42450267 8.08930639 8.31778577
Fe 8.07912492 8.87429632 8.32587804
Fe 8.12964654 11.35557647 8.34333697
Fe 11.43102312 8.88591775 6.30904586
Fe 11.44919964 11.29358736 6.32343789
Fe 14.27017437 10.04477019 9.40441274
S 12.33272136 10.09126477 10.44520550
S 10.11835075 10.52066812 12.01278437
Fe 9.77279619 10.12231103 2.67962061
Fe 7.65326522 10.12650930 3.95131035
Fe 5.57981060 10.13433272 5.28173770

Fe 8.52734677 14.12480305 5.28784807
Fe 9.83305528 14.11860277 7.44485279
Fe 11.25996577 14.33652199 9.47435007
Fe 8.44744065 6.11133486 5.26499733
Fe 9.71543253 6.07133693 7.41595977
Fe 11.09019485 5.87891320 9.51096994
Fe 6.21131181 7.53565071 9.53366301
Fe 6.37087056 10.15451940 9.61634507
Fe 6.28108937 12.76678478 9.49291063
Fe 13.15378079 7.59452171 5.23183259
Fe 13.24364980 10.08115920 5.26930456
Fe 13.20352088 12.55981080 5.25143942
S 7.84934847 8.72400060 10.46512187
S 7.87447016 11.57526036 10.47921238
Fe 13.59603177 8.78297534 7.38567999
Fe 13.62781372 11.32733877 7.39505622
Fe 5.93773821 8.91589326 7.43754036
Fe 5.97803708 11.36726130 7.44103214
Fe 11.48586135 8.84987892 3.92635891
Fe 11.50590644 11.35515401 3.93763340
Fe 12.63278103 12.11293703 9.61799886
S 10.65018540 12.48339960 10.50366831
Fe 9.13389828 12.14266336 3.95553926
Fe 7.00442901 12.17459513 5.31407314
Fe 12.56964238 8.04929415 9.58279862
S 10.54666519 7.82144924 10.45757294
Fe 9.10550962 8.09371462 3.93301070
Fe 6.95885336 8.08677652 5.29755084
Fe 7.50028830 13.40909811 7.44342214
Fe 8.82106091 13.38996614 9.65003622
Fe 7.41172291 6.84472548 7.43210944
Fe 8.70791290 6.83267023 9.64951042
Fe 10.88912006 13.40580285 5.29125309
Fe 12.21006304 13.31881942 7.41991177
Fe 10.82273632 6.79306242 5.27178739
Fe 12.13420137 6.81969465 7.40288551
C 13.10706557 12.41129882 11.53134335
C 13.88221351 10.05097846 11.50278378
C 13.71557761 11.31487255 12.23640662
C 11.12817882 13.89044757 11.61470711
C 12.26953881 13.28946425 12.31475226
C 8.65733938 13.92187026 11.55547769
C 9.86253956 14.10742665 12.32706531
C 6.59504283 12.53960756 11.54509851
C 7.51104135 13.42869811 12.27040016
C 5.81219372 10.17561537 11.50341795
C 5.96375876 11.41182210 12.23984957
C 6.54447978 7.80082949 11.58779105
C 5.95794602 8.95726190 12.26355652
C 8.54930305 6.35216784 11.57164695
C 7.45136110 6.91017204 12.32083695
C 11.02072654 6.26848709 11.56110537
C 9.76655580 6.11724382 12.30724232
C 13.04866596 7.70279720 11.46111314
C 12.19913271 6.81986124 12.22686295

C 13.69596759 8.76734058 12.19510880
C 12.23061435 13.23083646 13.74055164
C 13.72241275 11.26422955 13.66015499
C 13.10535980 12.31765609 14.42163620
C 9.86912103 14.04214541 13.75362172
C 11.09519265 13.75826191 14.47294685
C 7.48615712 13.39864595 13.69521598
C 8.62405770 13.85743975 14.44644216
C 5.93988726 11.43878762 13.65660688
C 6.54419709 12.54684206 14.37061751
C 5.96924929 8.96656525 13.69056899
C 5.75081010 10.20497818 14.37567846
C 7.47461156 6.98511881 13.74917995
C 6.59153894 7.89647037 14.43633332
C 9.80880664 6.18183116 13.73535900
C 8.60568308 6.46652123 14.47505258
C 12.21126087 6.82651926 13.65408937
C 11.07264604 6.35596969 14.41041703
C 13.74647963 8.76692258 13.61039847
C 13.14749079 7.67247282 14.33113470
C 13.95372609 10.01014452 14.32784630
C 11.07301136 13.67067150 15.89753972
C 13.09586788 12.25479770 15.84766283
C 12.18512696 13.06962255 16.60051696
C 8.60789220 13.80045390 15.87280944
C 9.83447654 13.88184194 16.61409524
C 6.49786316 12.56061327 15.78405445
C 7.43342698 13.34381543 16.55133549
C 5.70517104 10.22252655 15.78967715
C 5.81021599 11.49020231 16.45606734
C 6.61471543 7.95207019 15.86280699
C 5.96493167 9.03119608 16.54921366
C 8.64101198 6.54612993 15.90222603
C 7.53487444 7.13909006 16.61122718
C 11.10317680 6.40859871 15.83664524
C 9.88526750 6.32807321 16.59781113
C 13.20949580 7.65178774 15.74513959
C 12.28459401 6.86420478 16.51171601
C 14.01269946 9.98642757 15.73961053
C 13.90950416 8.71642997 16.40777860
C 13.75511833 11.17452646 16.51459813
C 9.81652547 13.82847223 18.04216331
C 12.18199171 13.01139716 18.02762967
C 11.06622069 13.60159415 18.73013986
C 7.41337552 13.29435285 17.98642149
C 8.57650563 13.63508949 18.76006257
C 5.73711398 11.51330331 17.84032698
C 6.42089319 12.50484951 18.61683390
C 5.97558603 9.07925412 17.98457227
C 5.67014204 10.31038932 18.61438676
C 7.55164463 7.19143238 18.04012788
C 6.68584636 8.09875887 18.75882906
C 9.91960008 6.37575206 18.02612761
C 8.67618500 6.59976501 18.72709934
C 12.32229393 6.90517616 17.94700587

C 11.16819877 6.56164232 18.73226653
C 13.99850730 8.68507358 17.79089929
C 13.32418319 7.69004645 18.56931364
C 13.75797067 11.11872268 17.94861864
C 14.07165178 9.88556566 18.57139390
C 13.05259567 12.09603970 18.73146765
C 6.70399008 9.64482123 20.76630356
C 7.54015503 10.12448265 21.86117685
C 6.13298675 10.61730388 19.92944672
C 6.59754171 11.98006324 19.93091881
C 8.01315782 11.51082254 21.86237835
C 7.64459515 12.40096297 20.76811480
C 8.33934499 7.81008223 22.08279251
C 7.73276035 7.42258094 20.86380458
C 6.87747992 8.31759158 20.18170409
C 8.31679359 9.14445227 22.55117228
C 10.56098146 8.37484971 22.54059083
C 11.76778017 8.67492339 21.83814016
C 9.67508288 9.44336892 22.99119426
C 12.24096027 10.06166691 21.83751759
C 10.11819665 10.73890967 22.99178872
C 11.47185297 11.03951473 22.53949988
C 13.16026651 8.21144913 19.88824946
C 13.62624589 9.57410473 19.88892768
C 9.94901563 6.66426459 20.85159746
C 8.69988840 6.64411953 20.12296470
C 9.71950724 7.33710837 22.07554028
C 11.16563399 6.84860223 20.15609485
C 12.12265918 7.78876775 20.73435450
C 13.06124370 10.54448279 20.73362568
C 12.87770187 11.87178184 20.15487442
C 9.22731902 11.80877227 22.55402502
C 12.03265680 12.76550782 20.85053659
C 11.05765588 13.54959388 20.12446789
C 11.44318070 12.37573889 22.07570995
C 10.06201811 12.84957188 22.08606119
C 9.81772271 13.52689490 20.86714204
C 8.59411193 13.34348151 20.18311446

$Fe_{49}S_6$ with CNT(6,6)

Fe 9.89416200 9.93175162 9.81251318
Fe 11.97242222 9.97617064 10.85529380
Fe 9.88838245 9.99626896 12.37120897
Fe 9.89785705 9.88603864 7.56873157
Fe 7.86318561 9.86012223 8.76843053
Fe 9.23929257 11.83561436 8.73115851
Fe 10.49546378 11.95924164 10.76347104
Fe 9.32450384 7.94909152 8.84665928
Fe 10.59766018 7.99758371 10.90022141
Fe 8.22248491 8.69422621 10.82594227
Fe 8.16578408 11.15763104 10.75775272
Fe 11.56772431 8.74278203 8.81884870
Fe 11.53631716 11.12724538 8.78406828
Fe 14.19656777 10.00452789 11.93415127

S 12.04001205 10.15389977 13.01077892
S 9.91344747 9.95426062 14.77247757
Fe 9.88129488 9.85454291 5.12276297
Fe 7.77840355 9.80270227 6.38091656
Fe 5.68943130 9.78690098 7.72135942
Fe 8.52240527 13.87591947 7.65844313
Fe 9.78806704 13.96712788 9.75574362
Fe 11.21296604 14.12273936 11.85978766
Fe 8.72320508 5.83751736 7.83977500
Fe 10.00725387 5.92101598 9.96755086
Fe 11.36724165 5.94019005 12.07408320
Fe 6.47482023 7.28981551 12.00020344
Fe 6.38241192 9.92353853 12.02878665
Fe 6.32354785 12.45245888 11.96359037
Fe 13.34438931 7.46865521 7.75361794
Fe 13.35619495 9.93475314 7.70281413
Fe 13.28184417 12.39423231 7.69051887
S 8.02353947 8.67951328 12.94387259
S 8.14895841 11.22427997 12.88838631
Fe 13.71920123 8.72415275 9.87445583
Fe 13.70249012 11.21969420 9.82864406
Fe 6.08091785 8.62637845 9.85653213
Fe 6.02823962 11.12789831 9.77679499
Fe 11.62262132 8.65195097 6.42723235
Fe 11.58005534 11.13905990 6.38985985
Fe 12.67486612 12.10062422 11.98746260
S 10.49509805 12.20321207 12.87857976
Fe 9.21895246 11.87589932 6.34477422
Fe 7.08558117 11.84643217 7.61489813
Fe 12.77633490 7.98550260 12.28593389
S 10.50978709 7.95331715 13.06233609
Fe 9.28219098 7.83869855 6.45954887
Fe 7.15477060 7.77403718 7.76109791
Fe 7.43027079 13.14095994 9.74750973
Fe 8.73010438 13.29174993 11.98397147
Fe 7.61349657 6.61226008 9.92109723
Fe 8.87814284 6.65932844 12.13844646
Fe 10.92381755 13.19715320 7.65624573
Fe 12.21265858 13.23383083 9.77886831
Fe 11.04631014 6.61192174 7.78233493
Fe 12.34713620 6.75283538 9.93395459
C 11.20543056 5.69652413 13.94519085
C 12.43889100 6.36195256 13.81853389
C 14.23768628 8.93075963 13.72048771
C 14.44880928 10.32149737 13.77576588
C 12.96984844 13.07812261 13.67591442
C 11.89174528 13.99370821 13.70765421
C 8.79017591 14.20889523 13.66464685
C 7.52619643 13.63983566 13.58268455
C 5.67769527 11.03999732 13.61080868
C 5.57449258 9.65498370 13.73415101
C 8.11070385 6.12139692 13.87459804
C 6.86661835 6.80242304 13.87633578
C 10.34573159 5.80498167 15.07116789
C 8.89042541 5.97316518 15.06164048

C 12.99999466 7.03143428 14.95413351
C 11.06426388 6.11738754 16.27423104
C 12.38071364 6.69130817 16.21745378
C 13.85113737 8.22695928 14.90886316
C 14.11663706 11.14132876 14.88763690
C 14.03817183 8.97453205 16.12999465
C 14.14978716 10.40723916 16.11921484
C 13.44535282 12.44191123 14.86334486
C 11.06194967 14.13712154 14.87775782
C 12.87798600 12.93550140 16.09881290
C 11.68164697 13.73797559 16.11303022
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C 6.93498124 13.02435288 14.74689083
C 8.85836352 14.03026545 16.05275570
C 7.53485883 13.44996400 15.98683856
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C 5.80958366 8.90701727 14.92915605
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C 6.45044318 7.58517560 15.01098380
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C 7.05498444 7.20318845 16.26082193
C 10.36338165 6.10577356 17.52539391
C 8.93916263 6.25679255 17.53508287
C 12.94601619 7.19011429 17.43408871
C 11.09233225 6.23419208 18.73928015
C 12.42214258 6.77330006 18.69196846
C 13.79806756 8.33730266 17.39061774
C 13.99489501 11.12307387 17.34763332
C 14.10899308 9.01543207 18.60194450
C 14.20706150 10.44736803 18.58135554
C 13.32822468 12.38419417 17.33985222
C 10.96402338 13.90187024 17.35343099
C 12.84114134 12.89944954 18.58074855
C 11.61002232 13.63281090 18.60562641
C 9.54610331 14.06473690 17.32778564
C 6.92340694 13.03960257 17.20621728
C 8.80726014 13.96355337 18.55123841
C 7.43586578 13.54691198 18.44687346
C 6.06842148 11.89440258 17.21644286
C 5.93813230 9.09551328 17.39933057
C 5.70653495 11.28904095 18.46398657
C 5.71958006 9.85133532 18.58784664
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C 13.05419906 7.21179973 19.89966688
C 12.52086049 6.77143938 21.15721914
C 11.16888636 6.24234651 21.20336392
C 13.92523038 8.35182164 19.85532486
C 14.13596231 11.18242587 19.79811131
C 14.28181283 9.04815957 21.06263915
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C 10.90160208 13.76656200 19.85101545
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C 11.57840854 13.48851579 21.08990101
C 9.47314208 13.90175719 19.83153334
C 6.75214390 13.19022952 19.60736488
C 8.72838047 13.56837663 21.03532026
C 7.36188659 13.26006086 20.89621942
C 5.85525300 12.07430345 19.61246923
C 5.91615401 9.24802612 19.87791148
C 5.85057438 10.08689082 21.05819339
C 5.87839329 11.49486665 20.91105212
C 6.61818242 7.98954893 19.95557415
C 7.13807674 7.52133850 21.22348657
C 8.30627735 6.65637241 21.24164380
C 7.92892224 9.59621487 23.98969927
C 7.72377910 8.24386610 23.53484649
C 6.33627781 9.59682849 22.28844461
C 6.85083643 8.26525437 22.39631969
C 7.04346156 10.43017442 23.22804640
C 9.99639762 7.72184310 24.23614406
C 8.77156179 7.35130236 23.59194801
C 10.24979281 9.06132143 24.65694268
C 9.18863898 10.05091749 24.43447905
C 13.80231745 9.19322032 23.51092368
C 14.02147199 10.57081275 23.49291813
C 12.67592279 8.64242642 24.23002963
C 11.64058932 9.49477997 24.74344162
C 11.90654582 10.90245570 24.73624946
C 13.13883271 11.40468973 24.24936701
C 13.97946314 8.42724900 22.29515271
C 14.28947418 11.22805570 22.23042667
C 11.03071330 6.94922884 23.58721646
C 10.46446193 6.30060566 22.42427027
C 9.05133908 6.52924999 22.43737198
C 13.09020733 7.30238672 22.33525985
C 12.32648341 7.41678471 23.55377411
C 9.54526855 11.43599886 24.10234481
C 10.86652936 11.83948976 24.31987792
C 7.42446784 11.74214698 22.84774078
C 6.74089433 12.28979099 21.74361415
C 13.53554498 12.47255324 22.22530502
C 8.74333299 12.22172731 23.17320092
C 10.81718208 13.31452156 22.31706427
C 12.87240530 12.59102219 23.46655370
C 11.47803408 12.84491936 23.47928098
C 9.39554394 13.13279365 22.24470969